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An Evaluation of Approximation Methods for Three Body Scattering Problems

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by

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ABSTRACT

The Born approximation and the Schwinger variational principle are applied to two one-dimensional three-body scattering problems. These problems are also solved exactly, and their solutions exhibit the physically interesting processes of elastic, inelastic, and exchange scattering. Comparison between the exact cross sections for these various processes with those obtained from the approximation methods serves to evaluate the range and validity of these methods. The results are then examined to determine which are of general applicability and which are peculiar to the specific problems studied.

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Chapter I

INTRODUCTION

In order to describe the phenomena which occur in the ionosphere, in gaseous discharges, in collisions between atoms or between electrons and atoms, a knowledge of the cross sections of various physical processes is required. Experimental determinations of these quantities is beset with many difficulties. In a large number of cases it is not possible to reproduce in the laboratory the conditions for which the values of the cross sections are desired. In other cases, the measurements made are a sum of the effects of different processes. Therefore it is important to extend the theoretical methods for calculating the individual cross sections.

No exact solution has as yet been obtained for a physical problem which involves many particles. The mathematical complexity of such problems requires the use of approximating procedures. These in turn must be studied to determine the reliability of the results obtained.

For two body collision problems, Rutherford scattering ¹ for example, an exact solution is known and the results obtained from the application of approximating procedures can be compared with the exact results. Thus in this case, as is well known, the Born approximation ² yields the exact scattering cross sections. In the absence of an exact solution to a problem, the evaluation of an approximation method has been carried out by comparing the results so obtained with the available experimental data or with the results determined by a numerical integration of the differential equations involved.

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1. N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, (Clarendon Press, Oxford, 1949). Second Edition, Chapter 3, Sections 1, 2.
 2. Ibid., Chapter 7, Section 1.

Bates, Fundaminsky, Leech and Massey³ consider the Born and Oppenheimer approximations and compare the results with experimental values. Jost and Pais⁴ study the Born approximation for a Yukawa potential and compare the results with numerical calculations. Dalitz⁵ on the other hand analyzes this same problem in the limit as the Yukawa potential approaches the Coulomb potential so that a comparison can be made to the well known Born and exact results for the latter potential.

Variational procedures which have been especially fruitful⁶ have been similarly evaluated. In particular, the Schwinger^{7,8} variational principle has received a great deal of attention in the literature. Its value has been further enhanced by the work of Kato⁹ who established upper and lower bounds for this principle for two body problems. The extension of this variational principle to three body problems was made by Borowitz and Friedman¹⁰. The Schwinger variational principle is formulated in terms of a Green's function which in practice leads to computational difficulties. A variational principle which is more amenable to calculation is the Hulthén¹¹ procedure as modified by Kohn¹². For two body problems Kohn (see footnotes 12,13) was able to establish a relationship between his procedure and the Schwinger variational principle. Kato¹⁴ has been able to

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3. D. R. Bates, A. Fundaminsky, J. W. Leech and H. S. W. Massey, Phil. Trans. Roy. Soc. A243, 93 (1950).
 4. R. Jost and A. Pais, Phys. Rev. 82, 840 (1951).
 5. R. H. Dalitz, Proc. Roy. Soc. A 206, 509 (1950).
 6. J. M. Blatt and J. D. Jackson, Phys. Rev. 76, 18 (1949).
 7. J. Schwinger, Hectographed Notes on Nuclear Physics, Harvard 1947 (unpublished).
 8. N. Marcuvitz, Sec. IIID, Recent Developments in the Theory of Wave Propagation, New York University, Institute of Mathematical Sciences (1949).
 9. T. Kato, Prog. of Th. Phys. 6, 394 (1951).
 10. S. Borowitz and B. Friedman, Phys. Rev. 82, 441 (1953).
 11. L. Hulthén, Kungl. Fysio, Sällskapet Lund Förhand 14, 21 (1944).
 12. W. Kohn, Phys. Rev. 74, 1763 (1948).
 13. W. Kohn, Phys. Rev. 84, 495 (1951).
 14. T. Kato, Phys. Rev. 80, 475, (1950).

exhibit the relations among the Schwinger, Kohn and Hulthén variational principles for two body problems.

Altshuler¹⁵ has applied the Schwinger variational principle to the study of the static field model of the hydrogen atom and compares the results with the numerical calculations of Chandrasekhar and Breen¹⁶ and the estimates of Massey and Moiseiwitsch¹⁷. Some of the difficulties and practical limitations which arise in a study of the application of variational principles to three body problems can be appreciated by considering the work of Massey and Moiseiwitsch. These authors compare the results obtained from the Hulthén, Kohn and Huang¹⁸ variational principles with the numerical calculations of Macdougall¹⁹ and of Morse and Allis²⁰. Because numerical results are not available, however, the effectiveness of the variational methods in dealing with exchange and polarization cannot be explored. The results obtained by Verde²¹ and by Troesch and Verde²² using Hulthén's variational principle are similarly restricted.

The approach to the problem of evaluating various approximation methods adopted here is to consider three body problems which can be solved exactly. Then the same problems can be treated by various methods of approximation and the results obtained in this way can be compared with the exact results. Wildermuth^{23,24} has constructed and solved a class of three body problems which can be used for this purpose. These problems are one-dimensional

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15. S. Altshuler, Phys. Rev. 89, 1278 (1953).
 16. S. Chandrasekhar and F. Breen, Astrophys. J. 103, 41 (1946).
 17. H. S. W. Massey and B. I. Moiseiwitsch, Proc. Roy. Soc. A 205, 483 (1951).
 18. S. S. Huang, Phys. Rev. 76, 477 (1949).
 19. J. Macdougall, Proc. Roy. Soc. A 136, 549 (1932).
 20. P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933).
 21. M. Verde, Helv. Phys. Acta, 22, 339 (1949).
 22. A. Troesch and M. Verde, Helv. Phys. Acta 24, 39 (1951).
 23. K. Wildermuth, Research Report CX-3, Math. Res. Gr., New York University (1952).
 24. K. Wildermuth, Z. f. Phys. 127, 92 (1949).

three body problems which exhibit all the essential physical phenomena such as elastic, exchange and inelastic scattering that occur in actual physical problems. These problems are mathematically tractable so that the physical situations can be explored in great detail. They also serve as a means of gaining some insight into real physical problems which are much more complex. One of the main goals of this study is to examine the results obtained to see which are of general validity and which are consequences of the specific problems studied.

Two problems will be considered. The first of these is a three body one-dimensional problem which involves distinguishable particles. Its exact solution the calculation of the various scattering cross sections and the application of the Born approximation, the Hulthén-Kohn and Schwinger variational principles make up the content of Chapter II. The second problem is again a three body one-dimensional problem but now identical particles are involved. In addition to elastic and inelastic scattering which also occur in the first problem exchange scattering is possible. The overall procedure that is followed for this problem is the same as for the preceding one. However, the methods of approximation can be applied in two distinct ways. The first is to take the perturbation in a symmetric form. The development of the approximations in this way is dealt with in Chapter III. The other approach is to take the perturbation in an asymmetric form. The application of this procedure which is the one most often found in the literature is the content of Chapter IV.

The extensive use of the Born approximation, especially in many particle problems, has led us to examine this procedure in some detail. Specifically, the Born expansion, which results when the procedure for obtaining the Born approximation is iterated, is studied. An important result is that the Born expansion is shown to converge whereas the Born approximation may have no

useful domain of applicability whatever. The second Born approximation which is a substantial correction to the Born approximation does however have a useful domain of applicability. Jost and Pais²⁵ obtain results similar in content to these but for lack of numerical results are unable to evaluate the significance of the contribution from the second Born approximation. The magnitude of the correction due to the second Born approximation is indicative of the rapidity of the convergence of the Born expansion. A similar result can be found in the work of Dalitz²⁶ who evaluated the Born expansion up to the third Born approximation. The calculation was carried out to show the convergence of the Born expansion but this could also be seen from the calculation of the second Born approximation.

The above result implies that in practice additional terms in the Born expansion must be calculated if useful results are to be obtained. Actually such calculations are not feasible and other methods, in particular, variational procedures are used.

The Schwinger and Hulthén-Kohn variational principles are applied to the two problems considered here. Trial functions are restricted to be those of the Born type because in general the Schwinger variational principle is mathematically tractable for such trial functions. However, in this case the Hulthén-Kohn variational principles yields the same results as the Born approximation²⁷. Nonetheless the study of this variational principle leads to a generalization to many body problems of the relation between this and Schwinger's variational principle which was first given by Kohn²⁸ for two body problems.

25. loc. cit.

26. loc. cit.

27. Kohn, loc. cit.

28. Ibid.

In Chapters II and III, the Schwinger variational principle is applied to the problem of distinguishable particles and to the problem involving identical particles. For Born trial functions, this principle was expected to yield results that included the second Born approximation^{29,30}. However, the problem treated in Chapter II shows that the variational calculations do not, even for very large energies, approach the exact or Born results. On the other hand for smaller values of the energy the variational results are excellent where the Born results are completely inadequate. The result, for the symmetric problem dealt with in Chapter III, is very interesting. Here both the Schwinger and Born results are good approximations to the exact values for the antisymmetric solution of the problem for large values of the energy. But now for smaller values of the energy the Born results are very good whereas the variational results become far less satisfactory. To summarize the situation, these two problems indicate that if Born type trial functions are used in the Schwinger variational principle, the results which are obtained may be equivalent to the second Born approximation in that range of the energy where it is a good approximation to the exact results but that outside this energy range the variational principle fails to extend the domain of usefulness of the Born results. Furthermore the variational and Born results may not have a common domain of agreement yet one may give excellent results just where the other is unreliable.

Chapter IV is a study of the symmetric problem formulated with an asymmetric perturbation. The main consideration here is to see whether or not exchange scattering can be properly treated by this approach to the problem. An iterative procedure—the Born expansion—is examined in detail and it is found that this method does not yield exchange effects. Only if

29. Schwinger, loc. cit.

30. Altshuler, loc. cit.

the resulting series is evaluated to obtain the analytic function it represents in its restricted domain of validity can exchange phenomena appear. Hence the Born expansion as an approximation method fails to yield any information about exchange scattering. This result is in contrast with that obtained by the same method for the symmetric perturbation formulation of the same problem. There each term in the Born expansion displayed the effects due to exchange.

A procedure due to Mott and Massey³¹ which was devised to take exchange scattering properly into account was also studied. It was found that if the initial state of the system is taken as a trial function, which is the procedure followed in the Born approximation, then spurious terms arise in the calculation of the exchange scattered wave. Since this procedure is an approximate one such terms yield contributions which assume unwarranted importance especially if the results are to be used in an iterative procedure. However, if trial functions are used which represent the initial state of the system when the interaction between the incident and bound particles is neglected then the spurious terms do not appear and the resulting approximation is also improved. These results are directly applicable to actual physical problems.

Chapter V is a discussion of the results obtained from the preceding sections. Its object is to point up those results which have general validity and those whose special character indicate the direction in which further study would be profitable.

31. Cf. Reference 1, Chapter 8, Section 2, 4.

Chapter II

DISTINGUISHABLE PARTICLES

2.1 Statement of the Problem

We shall consider a system composed of an "atom" and an incident particle. The "atom" consists of a nucleus with infinite mass and a bound particle with finite mass. In addition it will be assumed that the system is one-dimensional so that each of its constituents can be described in terms of a single coordinate.

The time independent Schroedinger equation for this system is

$$\left\{ -\frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} - 2B \delta(x_2) + V(x_1 x_2) \right\} \Psi(x_1 x_2) = E \Psi(x_1 x_2). \quad (2.1.1)$$

The time dependent factor has been taken to be $\exp(-iEt/\hbar)$. The potential energy of the bound particle is $-2B \delta(x_2)$ where B is a real positive constant and $\delta(x_2)$ is Dirac's delta function. $V(x_1 x_2)$ represents the energy of interaction between the incident particle 1 and the bound particle 2. Its explicit form will be given later. m_1 and m_2 are the masses of particles 1 and 2 respectively and \hbar is Planck's constant divided by 2π . The total energy of the system is E . Particle 1, the incident particle, does not interact with the nucleus--the center of force--and is thereby distinguished from particle 2. In what follows, units are chosen such that $\hbar = 1$ and $m_1 = m_2 = 1/2$.

The unperturbed equation which is obtained from (2.1.1) by setting $V(x_1 x_2)$ equal to zero is separable. As will be shown in section (2.2), particle 2 has but one bound state with energy $-B^2$ and all other states are in the continuum with positive energies. This is a consequence of the Dirac delta type potential. Furthermore the system is capable of exhibiting

both elastic and inelastic scattering. The latter is particularly simple and represents the ionization of the "atom." The short range of the delta function has as its counterpart in actual physical problems the short range nuclear forces.

Equation (2.1.1) will be considered in momentum space. The advantage of the momentum over the coordinate representation was first pointed out by Dirac³² and the subsequent work of others^{33,34,35} has demonstrated its usefulness for the consideration of scattering problems. To obtain the momentum representation of equation (2.1.1) let

$$V(x_1, x_2) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(k_1, k_2) \exp(ik_1 x_1 + ik_2 x_2) dk_1 dk_2. \quad (2.1.2)$$

Substitute this into (2.1.1) and multiply the resulting equation by $\exp(-ik_1' x_1 - ik_2' x_2)$. Then integrate over $-\infty < x_1 < +\infty$ and $-\infty < x_2 < +\infty$. Equation (2.1.1) becomes

$$(k_1^2 + k_2^2 - E)f(k_1, k_2) - \frac{B}{\pi} \int_{-\infty}^{+\infty} f(k_1, k_2) dk_2 + \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} (k_1, k_2 | V | k_1', k_2') dk_1' dk_2' f(k_1', k_2') = 0 \quad (2.1.3)$$

where

$$(k_1, k_2 | V | k_1', k_2') \equiv \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} V(x_1, x_2) \exp\{-i(k_1 - k_1')x_1 - i(k_2 - k_2')x_2\} dx_1 dx_2. \quad (2.1.4)$$

The identity (2.1.4) will henceforth be referred to as the interaction between the particles.

To prevent the notation from becoming too cumbersome we shall hence-

- 32. P.A.M. Dirac, Quantum Mechanics, Third Edition (Clarendon Press, Oxford, 1947).
- 33. W. Kohn, Phys. Rev. 74, 1763 (1948).
- 34. K. Wildermuth, cf. Reference 23.
- 35. W. Heisenberg, Z.f. Phys. 120, 513 (1943).

forth use a single integral sign to replace multiple ones. The multiplicity of integrations to be performed will be indicated by the number of variables of integration. The range of integration will always extend from $-\infty$ to $+\infty$ for all the variables of integration. Any deviation from this convention will be explicitly indicated.

To complete the mathematical description of the physical system, the interaction between the particles must be specified. This interaction will be chosen to be hermitian so that the eigenvalues of the Schroedinger equation are real and the form of the equation for the conservation of probability density will be preserved. The interaction assumed is

$$(k_1 k_2 | V | k'_1 k'_2) = A \left\{ \frac{1}{(k_1 + iT)(k'_2 - iT)} + \frac{1}{(k_2 + iT)(k'_1 - iT)} \right\}, \quad (2.1.5)$$

where A and T are real constants. It follows from (2.1.5) that

$$(k_1 k_2 | V | k'_1 k'_2) = (k'_1 k'_2 | V | k_1 k_2)^*, \quad (2.1.6)$$

where the asterisk denotes the complex conjugate of the quantity so modified.

The form of the interaction (2.1.5) is dictated by the following considerations: Equation (2.1.3) is readily solved if the last term on the left hand side can be evaluated. This can be done by taking the interaction to be a product of the form $V(k_1 k_2) V(k'_1 k'_2)^*$. Another important property of the interaction is that when expressed in coordinate space it should vanish rapidly for large separations between the "atom" and the incident particle. This is satisfied by (2.1.5). In coordinate space this interaction is an integral operator with a kernel given by

$$A \left[\delta(x_2) \eta(-x_1) \exp(Tx_1) \delta(x_1) \eta(-x_2) \exp(Tx_2) \right. \\ \left. + \delta(x_1) \eta(-x_2) \exp(Tx_2) \delta(x_2) \eta(-x_1) \exp(Tx_1) \right] ,$$

where

$$\eta(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} .$$

This interaction is evidently one which vanishes rapidly for large distances x_1 and/or x_2 . Physically, the two particles interact only when one of them is at the origin and the other is to the left of the origin. The interaction between them is greatest when the particles are at the origin.

The interaction (2.1.5) may be further simplified to a product of two factors. However, in that case, the Schwinger variational principle gives the exact solution for arbitrary trial functions. To make this principle depend on the choice of trial functions a sum of such products must be chosen.

The physical problem which is mathematically represented by equation (2.1.3) and the identity (2.1.5) is the following: Particle 1 is incident from the left with momentum K_0 and interacts with the "atom." Since it does not interact with the center of force, exchange scattering is impossible, but it does undergo elastic and inelastic scattering. The exact wave function and the cross sections for elastic and inelastic scattering are to be determined.

These cross sections are also to be calculated from the Born approximation, the Hulthén-Kohn variational principle and the Schwinger variational principle. The comparison of these results with the exact result will enable us to evaluate these approximating procedures.

2.2 Mathematical Preliminaries

Equation (2.1.3) with the interaction (2.1.5) can be solved in various ways. For purposes of reference, the methods of solution will be designated:

the direct method, the expansion method and the Green's function technique. All these methods of course lead to the same result but the details of each method will be found useful when the various methods of approximation are considered.

2.2.1 The Direct Method

Initially particle 1 and the "atom" are so far apart that the interaction between them is negligible. The initial state of the system is then a solution of the unperturbed Schroedinger equation

$$(k_1^2 + k_2^2 - E) f_0(k_1 k_2) - (B/\pi) \int f_0(k_1 k_2) dk_2 = 0, \quad (2.2.1)$$

which is obtained from equation (2.1.3) by setting the interaction equal to zero. This equation when transcribed to coordinate space is separable and its solution is straightforward. It is also separable in momentum space and its solution may be readily obtained by exploiting the physical situation which it represents.

Since particle 1 is incident from the left with momentum K_0 and does not interact with the center of force or with the bound particle 2 it must proceed undisturbed. The state of particle 1 is described by a plane wave $(2\pi)^{-1/2} \exp(iK_0 x_1)$ in coordinate space which is represented by $\delta(k_1 - K_0)$ in momentum space. The normalization of the plane wave was chosen as indicated purely as a matter of convenience. The momentum representation is easily verified by substituting it into the one-dimensional equivalent of (2.1.2). Therefore the solution of (2.2.1) has the form

$$f_0(k_1 k_2) = \delta(k_1 - K_0) f(k_2), \quad (2.2.2)$$

where $f(k_2)$ must represent the bound state of particle 2 since the latter is undisturbed by the passage of particle 1. The energy of particle 1 is

K_0^2 , whence the energy of particle 2 must be $E_2 = E - K_0^2$, where E is the total energy of the system. Substitute (2.2.2) into (2.2.1). Then we find that $f(k_2)$ must satisfy

$$(k_2^2 - E_2) f(k_2) - (B/\pi)D = 0, \quad (2.2.3)$$

where the constant

$$D = \int f(k_2) dk_2. \quad (2.2.4)$$

From (2.2.3) and the requirement that $f(k_2)$ represents a bound state, it follows that

$$f(k_2) = (B/\pi) D / (k_2^2 - E_2), \quad (2.2.5)$$

provided that $E_2 < 0$. From (2.2.4) and (2.2.5)

$$D = BD / (-E_2)^{1/2}.$$

The only solution is that for which $E_2 = -B^2$, where the positive square root must be taken since B is positive. The constant D which appears to be arbitrary is fixed by the normalization of $f(k_2)$. Hence the solution of the unperturbed Schrodinger equation (2.2.1) has only one bound state with negative energy for particle 2. This bound state is given by

$$f(k_2) = N / (k_2^2 + B^2), \quad (2.2.6)$$

where

$$N = (2/\pi)^{1/2} B^{3/2} \quad (2.2.7)$$

N is a constant determined from the normalization of $f(k_2)$. Combining equations (2.2.6) and (2.2.2) we find that the solution to equation (2.2.1) is

$$f_0(k_1 k_2) = \delta(k_1 - K_0) N / (k_2^2 + B^2) \quad (2.2.8)$$

with

$$N = (2/\pi)^{1/2} B^{3/2} \quad \text{and} \quad K_0^2 = B^2 + E. \quad (2.2.9)$$

Now represent the solution of equation (2.1.3) as

$$f(k_1 k_2) = f_0(k_1 k_2) + f_1(k_1 k_2), \quad (2.2.10)$$

where $f_0(k_1 k_2)$ is the solution (2.2.8) of the unperturbed equation (2.2.1) and $f_1(k_1 k_2)$ represents the outgoing flux of particles which results from the interaction between the incident and bound particles. Substitute (2.2.10) into equation (2.1.3). Then we find that $f_1(k_1 k_2)$ must satisfy

$$(k_1^2 + k_2^2 - E) f_1(k_1 k_2) - F(k_1) + \frac{A}{4\pi^2} \left\{ \frac{C}{k_1 + iT} + \frac{D}{k_2 + iT} \right\} = 0, \quad (2.2.11)$$

in which

$$F(k_1) = (B/\pi) \int f_1(k_1 k_2) dk_2 \quad (2.2.12)$$

and

$$C = \int dk_1 dk_2 f(k_1 k_2) / (k_2 - iT), \quad (2.2.13)$$

$$D = \int dk_1 dk_2 f(k_1 k_2) / (k_1 - iT).$$

From (2.2.11) we obtain

$$f_1(k_1 k_2) = \left[F(k_1) - \frac{A}{4\pi^2} \left\{ \frac{C}{k_1 + iT} + \frac{D}{k_2 + iT} \right\} \right] \frac{1}{k_1^2 + k_2^2 - E}. \quad (2.2.14)$$

In this equation it is to be understood that a small positive imaginary part (see footnotes 23, 26, 28) has been added to the total energy E to insure that $f_1(k_1 k_2)$ represents outgoing waves in coordinate space. A singularity of the delta function type does not appear in (2.2.14) because the condition on $f_1(k_1 k_2)$ is that it represents outgoing waves only. $F(k_1)$ can be evaluated by substituting (2.2.14) into (2.2.12). Then

$$f_1(k_1 k_2) = - \frac{A}{4\pi^2} \left[\frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} \frac{C}{k_1 + iT} + D \left\{ \frac{Bi}{(\sqrt{E - k_1^2} - Bi)(\sqrt{E - k_1^2} + iT)} + \frac{1}{k_2 + iT} \right\} \right] \frac{1}{k_1^2 + k_2^2 - E} \quad (2.2.15)$$

The constants C and D are determined from the evaluation of (2.2.13).

Their values are

$$C = \frac{N\pi}{B} \left\{ \frac{1}{B+T} \left(1 - \frac{A}{4\pi} J_1 i \right) - \frac{A}{4\pi (K_0 - iT)} (BJ_2 + iJ_3) \right\} \Delta, \quad (2.2.16)$$

$$D = \frac{N\pi}{B} \left\{ \frac{1}{K_0 - iT} \left(1 - \frac{A}{4\pi} J_1 i \right) + \frac{iA}{4\pi (B+T)} - \frac{J_4}{T} \right\} \Delta,$$

where

$$\Delta^{-1} = \left(1 - \frac{A}{4\pi} J_1 i \right)^2 + \left(\frac{A}{4\pi} \right)^2 \frac{J_4}{T} (BJ_2 + iJ_3), \quad (2.2.17)$$

and J_i , ($i = 1, 2, 3, 4$) are functions of the total E and the constants B and T . The explicit expressions for these functions will be found in Appendix I.

From (2.2.15) and (2.2.10) we find that the exact solution to equation (2.1.3) for the interaction (2.1.5) is

$$f(k_1 k_2) = \frac{\delta(k_1 - K_0) N}{(k_2^2 + B^2)} - \frac{A}{4\pi^2} \frac{1}{k_1^2 + k_2^2 - E} \times \quad (2.2.18)$$

$$\left[\frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} - \frac{C}{k_1 + iT} + D \left\{ \frac{Bi}{(\sqrt{E - k_1^2} - Bi)(\sqrt{E - k_1^2} + Ti)} + \frac{1}{k_2 + iT} \right\} \right].$$

2.2.2 The Expansion Method

The solution of equation (2.1.3) can be found by expanding it in terms of the eigenfunctions of the unperturbed Schroedinger equation

$$(k_1^2 + k_2^2 - E) g(k_1 k_2) - (B/\pi) \int g(k_1 k_2) dk_2 = 0. \quad (2.2.19)$$

The eigenfunctions of this equation are to be determined subject to the condition that they represent incident plus outgoing waves. To obtain these eigenfunctions, equation (2.2.19) can be solved in a manner analogous to the solution of equation (2.2.1). Thus one of the eigenfunctions of (2.2.19) is

$$(K_1 \neq |k_1 k_2) \equiv \delta(k_1 - K_1) N / (k_2^2 + B^2) \quad (2.2.20)$$

with $K_1^2 = B^2 + E$. K_1 is the momentum of the incident particle 1. The other eigenfunction is obtained from equation (2.2.3) which when written in our present notation becomes

$$(k_2^2 - K_2^2) g(k_2) - (B/\pi) D = 0, \quad (2.2.21)$$

where $K_2^2 = E - K_1^2$ and

$$D = \int g(k_2) dk_2. \quad (2.2.22)$$

The solution of (2.2.21) which satisfies the conditions of the problem

is

$$g(k_2) = \delta(k_2 - K_2) + \frac{B}{\pi} \frac{D}{k_2^2 - K_2^2 - i\alpha}. \quad (2.2.23)$$

A small positive imaginary part $i\alpha$ ($\alpha > 0$) has been added to the total energy E to insure that the last term on the right hand side of (2.2.23) represents outgoing waves in coordinate space. Throughout the remainder of this work when outgoing waves are considered it will be understood that the total energy E will have associated with it a small positive imaginary part.

The constant D is determined by substituting (2.2.23) into (2.2.22) and carrying out the indicated integration. In this way we find that the second eigenfunction is

$$(K_1 K_2 | k_1 k_2) \equiv \delta(k_1 - K_1) \left\{ \delta(k_2 - K_2) + \frac{B}{\pi} \frac{|K_2|}{|K_2| - B i} \frac{1}{k_2^2 - K_2^2 - i\alpha} \right\} \quad (2.2.24)$$

with $K_1^2 + K_2^2 = E$.

The eigenfunctions (2.2.20) and (2.2.24) satisfy the orthogonality relations

$$\int (K_1' K_2' | k_1 k_2)^* dk_1 dk_2 (K_1 K_2 | k_1 k_2) = \delta(K_1 - K_1') \delta(K_2 - K_2'), \quad (2.2.25)$$

$$\int (K_1' 2 | k_1 k_2)^* dk_1 dk_2 (K_1 2 | k_1 k_2) = \delta(K_1 - K_1')$$

$$\int (K_1 K_2 | k_1 k_2)^* dk_1 dk_2 (K_1' 2 | k_1 k_2) = 0$$

The closure property is also satisfied, i.e.,

$$\begin{aligned} \int (K_1 K_2 | k_1' k_2')^* dK_1 dK_2 (K_1 K_2 | k_1 k_2) + \int (K_1 2 | k_1' k_2')^* dK_1 (K_1 2 | k_1 k_2) \\ = \delta(k_1 - k_1') \delta(k_2 - k_2') \end{aligned} \quad (2.2.26)$$

Equations (2.2.25) and (2.2.26) assert that the eigenfunctions (2.2.20) and (2.2.24) constitute a complete set.

To solve equation (2.1.3) we let

$$f(k_1 k_2) = f_0(k_1 k_2) + f_1(k_1 k_2), \quad (2.2.27)$$

with the same significance attached to $f_0(k_1 k_2)$ and $f_1(k_1 k_2)$ as was given to them below equation (2.2.10). Then $f_1(k_1 k_2)$ must satisfy

$$(k_1^2 + k_2^2 - E) f_1(k_1 k_2) - (B/\pi) \int f_1(k_1 k_2) dk_2 + V(k_1 k_2) = 0, \quad (2.2.28)$$

in which

$$V(k_1 k_2) \equiv (1/4\pi^2) \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f(k_1' k_2'). \quad (2.2.29)$$

Now expand $f_1(k_1 k_2)$ in terms of the eigenfunctions of the unperturbed equation. Then

$$f_1(k_1 k_2) = \int f(K_1) dK_1 (K_1 2 | k_1 k_2) + \int f(K_1 K_2) dK_1 dK_2 (K_1 K_2 | k_1 k_2), \quad (2.2.30)$$

where $f(K_1)$ and $f(K_1 K_2)$ are the expansion coefficients. These are different functions but to simplify the notation their arguments are used to distinguish between them. Substitute (2.2.30) into (2.2.28). Then the latter equation becomes

$$\begin{aligned} & \int (k_1^2 + k_2^2 - E) f(K_1) dK_1 (K_1 \rightarrow k_1 k_2) - (B/\pi) \int f(K_1) dK_1 (K_1 \rightarrow k_1 k_2) dk_2 \\ & + \int (k_1^2 + k_2^2 - E) f(K_1 K_2) dK_1 dK_2 (K_1 K_2 \rightarrow k_1 k_2) - (B/\pi) \int f(K_1 K_2) dK_1 dK_2 (K_1 K_2 \rightarrow k_1 k_2) dk_2 \\ & = -V(k_1 k_2). \end{aligned} \quad (2.2.31)$$

Since

$$(k_1^2 + k_2^2 - K_1^2 - K_2^2) (K_1 K_2 \rightarrow k_1 k_2) - (B/\pi) \int (K_1 K_2 \rightarrow k_1 k_2) dk_2 = 0,$$

and

$$(k_1^2 + k_2^2 - K_1^2 + B^2) (K_1 \rightarrow k_1 k_2) - (B/\pi) \int (K_1 \rightarrow k_1 k_2) dk_2 = 0,$$

equation (2.2.31) reduces to

$$\begin{aligned} & \int (K_1^2 - B^2 - E) f(K_1) dK_1 (K_1 \rightarrow k_1 k_2) \\ & + \int (K_1^2 + K_2^2 - E) f(K_1 K_2) dK_1 dK_2 (K_1 K_2 \rightarrow k_1 k_2) = -V(k_1 k_2). \end{aligned} \quad (2.2.32)$$

Multiply this equation with $(K_1 \rightarrow k_1 k_2)^* dk_1 dk_2$ and $(K_1 K_2 \rightarrow k_1 k_2)^* dk_1 dk_2$ in turn and integrate over the indicated variables. Then the following two equations,

$$(K_1^2 - K_0^2) f(K_1) = - \int (K_1 \rightarrow k_1 k_2)^* dk_1 dk_2 V(k_1 k_2); K_0^2 = B^2 + E$$

and

$$(K_1^2 + K_2^2 - E) f(K_1 K_2) = - \int (K_1 K_2 \rightarrow k_1 k_2)^* dk_1 dk_2 V(k_1 k_2) \quad (2.2.33)$$

result when the orthogonality relations (2.2.25) are used. Since $f(K_1)$

and $f(K_1 K_2)$ are to represent outgoing waves, it follows that

$$f(K_1) = - \frac{1}{K_1^2 - K_0^2} \int (K_1 \rightarrow k_1 k_2)^* dk_1 dk_2 V(k_1 k_2)$$

and

(2.2.34)

$$f(K_1 K_2) = - \frac{1}{K_1^2 + K_2^2 - E} \int (K_1 K_2 \rightarrow k_1 k_2)^* dk_1 dk_2 V(k_1 k_2).$$

When equations (2.2.34) are substituted into (2.2.30) we find that

$$f_1(k_1 k_2) = - \int \left[\frac{(K_1 K_2 | k_1' k_2')^* dK_1 dK_2 (K_1 K_2 | k_1 k_2)}{K_1^2 + K_2^2 - E} + \frac{(K_1 2 | k_1' k_2')^* dK_1 (K_1 2 | k_1 k_2)}{K_1^2 - K_0^2} \right] dk_1' dk_2' V(k_1' k_2') \quad (2.2.35)$$

The evaluation of the right side of this equation yields the same expression for $f_1(k_1 k_2)$ as obtained by the direct method--equation (2.2.15).

2.2.3 The Green's Function Technique

The Green's function for equation (2.1.3) is that solution of

$$(k_1^2 + k_2^2 - E)G(k_1 k_2; k_1' k_2') - (B/\pi) \int G(k_1 k_2; k_1' k_2') dk_2 = \delta(k_1 - k_1') \delta(k_2 - k_2'), \quad (2.2.36)$$

which represents outgoing waves in coordinate space. This equation can be solved by either of the previous methods discussed. The expansion method gives the result immediately, for $G(k_1 k_2; k_1' k_2')$ satisfies the same conditions as $f_1(k_1 k_2)$. Thus to obtain the Green's function from (2.2.35) we need only replace $V(k_1 k_2)$ by $-\delta(k_1 - k_1') \delta(k_2 - k_2')$. It follows that

$$G(k_1 k_2; k_1' k_2') = \int \frac{(K_1 K_2 | k_1' k_2')^* dK_1 dK_2 (K_1 K_2 | k_1 k_2)}{K_1^2 + K_2^2 - E} + \int \frac{(K_1 2 | k_1' k_2')^* dK_1 (K_1 2 | k_1 k_2)}{K_1^2 - K_0^2} \quad (2.2.37)$$

On evaluating these integrals we find that

$$G(k_1 k_2; k_1' k_2') = \frac{\delta(k_1 - k_1')}{k_1^2 + k_2^2 - E} \left[\frac{B}{\pi} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} \frac{1}{k_1^2 + k_2^2 - E} + \delta(k_2 - k_2') \right] \quad (2.2.38)$$

Both of these forms for the Green's function will be needed in the work which follows.

It is important to note that equation (2.2.38) gives the relation

$$G(k_1 k_2; k'_1 k'_2) = G(k'_1 k'_2; k_1 k_2). \quad (2.2.39)$$

This symmetry between the unprimed and primed momenta is not apparent in equation (2.2.37). However, both the orthogonality and closure relationships are symmetric in the interchange of the eigenfunctions with its complex conjugate. Therefore the expansion may be made in terms of the complex conjugates of the eigenfunction. In that event equation (2.2.37) would display the property given by equation (2.2.39).

The solution of equation (2.2.36) by the direct method leads directly to equation (2.2.38), so that there is no need to repeat the details.

Once the Green's function has been determined, the solution to equation (2.1.3) may be represented by the following integral equation.

$$(2.2.40)$$

$$f(k_1 k_2) = f_0(k_1 k_2) - (1/4\pi^2) \int G(k_1 k_2; k'_1 k'_2) dk'_1 dk'_2 (k'_1 k'_2 | V | k_1 k_2) dk'_1 dk'_2 f(k'_1 k'_2).$$

The integral on the right hand side is identical with that obtained for $f_1(k_1 k_2)$ and given by equation (2.2.35). In (2.2.35) the term in the square brackets is just the Green's function and the definition (2.2.29) of $V(k_1 k_2)$ completes the identification. Thus the integral equation formulation of the problem leads automatically to the exact solution.

2.3 The Exact Solution

The solution to equation (2.1.3) given by (2.2.18) represents the state of the system in momentum space. To obtain the solution in coordinate space equation (2.2.18) must be inserted into (2.1.2) and the resulting integral evaluated. The wave function in coordinate space describes the state of the system for all values of the coordinates x_1 and x_2 . This information is

much more than we require. We are interested in the scattered wave in coordinate space, i.e., for large values of x_1 and/or x_2 . Therefore only that part of the wave function in momentum space which contributes to the scattered wave in coordinate space is of interest. This part of the wave function in momentum space can be separated from that portion which describes the system when the particles are close to each other by applying the Riemann-Lebesgue theorem³⁶. This theorem states that if $f(k)$ is bounded and integrable over the range of integration, say, $a \leq k \leq b$, then

$$\lim_{x \rightarrow \infty} \int_a^b f(k) \exp(ikx) dk = 0. \quad (2.3.1)$$

An immediate consequence of this theorem is that non-zero contributions from integrals of the form given in (2.3.1) for large values of x come from those regions of the variable of integration where $f(k)$ is unbounded, i.e., at the singularities of $f(k)$. Since the range of momenta is over the real axis, the singularities that are important are those that lie on the real axis. Therefore to obtain the scattered wave in coordinate space all that need be known is the value of the wave function at its singularities on the real axis of momentum space. The value of the wave function at its singularities on the real axis of momentum space will be referred to as the asymptotic part of the wave function.

The asymptotic part of the exact solution $f(k_1 k_2)$ is

$$\begin{aligned} f(k_1 k_2) \sim & \delta(k_1 - K_c) \frac{N}{k_2^2 + B^2} - \frac{A}{4\pi^2} \frac{N\pi}{B} \left[\frac{C}{k_1 + iT} + \frac{D}{i(E+T)} \right] \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 - K_0^2} \\ & - \frac{A}{4\pi^2} \frac{1}{k_1^2 + k_2^2 - E} \left[\frac{|k_2|}{|k_2| - Bi} \frac{C}{k_1 + iT} + D \left\{ \frac{Bi}{(|k_2| - Bi)(|k_2| + iT)} + \frac{1}{k_2 + iT} \right\} \right] \end{aligned} \quad (2.3.2)$$

The tilde denotes that the asymptotic part of the function is to follow.

The first term on the right hand side of the equation (2.3.2) represents

36. H. S. Carslaw, Introduction to the Theory of Fourier's Series and Integrals (Dover Publications, 1930). Third Edition.

the initial state of the system. The second and third terms represent the effect of the interaction on the initial state of the system. To examine the significance of the second and third terms, $f(k_1 k_2)$ is expressed in a mixed representation in which particle 1 is described in coordinate space and particle 2 is described in momentum space. This representation is obtained by evaluating (2.1.2) only for the integration over k_1 . The result is

$$F(x_1, k_2) = \begin{cases} \frac{1}{(2\pi)^{1/2}} \frac{N}{k_2^2 + B^2} \exp(iK_0 x_1) + \frac{aN}{k_2^2 + B^2} \exp(iK_0 x_1) + b \exp\left\{i(E-k_2^2)^{1/2} x_1\right\}; & (x_1 > 0) \\ \frac{1}{(2\pi)^{1/2}} \frac{N}{k_2^2 + B^2} \exp(iK_0 x_1) + \frac{cN}{k_2^2 + B^2} \exp(-iK_0 x_1) + d \exp\left\{-i(E-k_2^2)^{1/2} x_1\right\}; & (x_1 < 0) \end{cases} \quad (2.3.3)$$

where

$$\begin{aligned} a &= -\frac{A}{4\pi^2} \frac{N\pi}{B} \frac{\pi i}{K_0} \frac{1}{(2\pi)^{1/2}} \left[\frac{C}{K_0 + iT} + \frac{D}{i(B+T)} \right] \\ b &= -\frac{A}{4\pi^2} \frac{\pi i}{(2\pi)^{1/2}} \frac{1}{(E-k_2^2)^{1/2}} \left[\frac{|k_2|}{(|k_2| - Bi)} \frac{C}{(\sqrt{E-k_2^2} + iT)} + D \left\{ \frac{Bi}{(|k_2| - Bi)(|k_2| + iT)} \right. \right. \\ &\quad \left. \left. + \frac{1}{k_2 + iT} \right\} \right] \\ c &= -\frac{A}{4\pi^2} \frac{N\pi}{B} \frac{\pi i}{K_0} \frac{1}{(2\pi)^{1/2}} \left[-\frac{C}{K_0 - iT} + \frac{D}{i(B+T)} \right] \\ d &= -\frac{A}{4\pi^2} \frac{\pi i}{(2\pi)^{1/2}} \frac{1}{(E-k_2^2)^{1/2}} \left[-\frac{|k_2|}{(|k_2| - Bi)} \frac{C}{(\sqrt{E-k_2^2} - iT)} + D \left\{ \frac{Bi}{(|k_2| - Bi)(|k_2| + iT)} \right. \right. \\ &\quad \left. \left. + \frac{1}{k_2 + iT} \right\} \right]. \end{aligned} \quad (2.3.4)$$

The one dimensional character of this problem is indicated by equation (2.3.3) where $F(x_1 k_2)$ is given for forward ($x_1 > 0$) and backward ($x_1 < 0$) scattering. This replaces the angular dependence which arises in three dimensional problems. The first terms in (2.3.3) represent the incident wave and arise from the factor $\delta(k_1 - K_0)$ in momentum space. The second terms arise from the factor $1/(k_1^2 - K_0^2)$ and express outgoing waves with momentum K_0 in the forward and backward directions. These outgoing waves are the result of elastic collisions since the energy of these particles remains the same. The third terms which arise from the factor $1/(k_1^2 + k_2^2 - E)$ also represent outgoing waves but with momentum $|k_1| = \sqrt{E - k_2^2}$. These waves are the result of inelastic collisions since the energy of these particles has been altered. The contributions to the inelastically scattered waves are limited to values such that $E - k_2^2 > 0$, for otherwise these scattered waves drop off exponentially. It is evident that the contributions to the scattered waves come from those values of the momenta which satisfy the principle of the conservation of energy. Of course the physics of the situation demands this. If $E < 0$ there is no inelastically scattered wave and this again represents the physical situation, for it is then energetically impossible for both particles to be scattered.

The cross sections for elastic and inelastic scattering can now be determined. Consider the inelastically scattered wave in equation (2.3.3). The coefficient of the exponential term is the probability amplitude and its absolute value squared gives the probability of finding particle 1 at x , with momentum $|k_1| = \sqrt{E - k_2^2}$ when particle 2 has momentum in the range between k_2 and $k_2 + dk_2$. The total outgoing current density is then given by

$$\int_{-\sqrt{E}}^{+\sqrt{E}} \frac{|k_1|}{m_1} \left\{ |b|^2 + |d|^2 \right\} dk_2 \quad (2.3.5)$$

The total incoming current density of particles 1 is determined from the probability amplitude of the incident wave and is

$$\int \frac{K_0}{m_1} \left[\frac{1}{(2\pi)^{1/2}} \frac{1}{k_2^2 + B^2} \right]^2 dk_2 = K_0/\pi \quad (2.3.6)$$

The cross section for inelastic scattering is obtained by dividing (2.3.5) by (2.3.6) and this is

$$Q_i = \frac{2\pi}{K_0} \int_{-\sqrt{E}}^{\sqrt{E}} |k_1| \left\{ |b|^2 + |d|^2 \right\} dk_2 \quad (2.3.7)$$

In a similar manner the cross section for elastic scattering can be found and it is given by

$$Q_e = 2\pi \left\{ |a|^2 + |c|^2 \right\} \quad (2.3.8)$$

Substitute the values for a, b, c, and d given by (2.3.4) into (2.3.7) and (2.3.8). Then the cross sections become equal to

$$\begin{aligned} Q_i = & \frac{A^2}{8\pi K_0} \left[\frac{|c|^2}{K_0^2 + T^2} \left\{ \frac{(T^2 + E)^{1/2}}{T} - \frac{B}{(B^2 + E)^{1/2}} \right\} \right. \\ & - \frac{T}{(B+T)(K_0^2 + T^2)} \left\{ \frac{B}{(B^2 + E)^{1/2}} - \frac{2T^4 + 2T^2 E - B^2 E}{(2T^2 + E)T(T^2 + E)^{1/2}} \right\} \left\{ CD^* + C^* D \right\} \\ & \left. + |D|^2 \left\{ \frac{BE}{T(T+B)(T^2 + E)^{3/2}} + \frac{T}{(T+B)^2(T^2 + E)^{1/2}} - \frac{B}{(T+B)^2(B^2 + E)^{1/2}} \right\} \right] \end{aligned} \quad (2.3.9)$$

for $E > 0$, and

$$Q_e = \frac{A^2 B}{4\pi K_0^2} \left[\frac{|c|^2}{K_0^2 + T^2} + \frac{T}{(B+T)(K_0^2 + T^2)} \left\{ CD^* + C^* D \right\} + \frac{|D|^2}{(B+T)^2} \right]. \quad (2.3.10)$$

From (2.3.9) it is easy to verify that $Q_i = 0$ for $E = 0$ whatever the values C and D might have. Physically this is necessary since on energetic considerations alone the inelastic scattering cross section must vanish for all values of the total energy which is less than or equal to zero. The values for C and D should in no way affect this basic physical requirement.

It is clear from equations (2.3.9) and (2.3.10) that the cross sections depend on the constants C and D. The approximation procedures considered below are used to determine the values of these constants.

The continuity equation for the probability density leads to the following relation between the scattering cross sections

$$Q_e + Q_i = - \frac{A}{4\pi} \frac{N\pi}{B} \frac{2}{K_0} \operatorname{Im} \left\{ \frac{C}{K_0 + iT} + \frac{D}{i(B+T)} \right\} \quad (2.3.11)$$

This relation is an instance of a general theorem³⁷ which relates the total cross section for scattering to the imaginary part of the probability amplitude of the wave scattered elastically in the forward direction. This equation has been independently checked by inserting the values for C and D and comparing the coefficients of like powers of the independent parameter A. The right hand side of equation (2.3.11) may be used to calculate the total cross section but we are interested in the individual cross sections. Nevertheless equation (2.3.11) serves as a useful check on the numerical calculations and has been used for this purpose.

2.4 The Born Approximation

Consider equation (2.1.3) written in the following way,

(2.4.1)

$$(k_1^2 + k_2^2 - E)f(k_1, k_2) - (B/\pi) \int f(k_1, k_2) dk_2 = -(1/4\pi^2) \int (k_1, k_2 | V | k'_1, k'_2) dk'_1 dk'_2 f(k'_1, k'_2) .$$

The Born approximation to the exact solution is obtained by solving the equation which results when $f(k_1, k_2)$ in the integral on the right hand side of the above equation is replaced by that solution of the unperturbed equation which represents the initial state of the system. The unperturbed equation

37. B. A. Lippman and J. Schwinger, Phys. Rev. 79, 469 (1950).

is the left hand side of (2.4.1) equated to zero and is the same equation as (2.2.1). Its solution is

$$f_0(k_1 k_2) = \delta(k_1 - K_0) N / (k_2^2 + B^2). \quad (2.4.2)$$

The Born approximation, $f^{(1)}(k_1 k_2)$, to the exact solution satisfies the equation, (2.4.3)

$$(k_1^2 + k_2^2 - E) f^{(1)}(k_1 k_2) - (B/\pi) \int f^{(1)}(k_1 k_2) dk_2 = - \frac{A}{4\pi^2} \left\{ \frac{C_B}{k_1 + iT} + \frac{D_B}{k_2 + iT} \right\},$$

where

$$C_B = \int dk_1 dk_2 f_0(k_1 k_2) / (k_2 - iT) = N\pi / B(T+B) \quad (2.4.4)$$

and

$$D_B = \int dk_1 dk_2 f_0(k_1 k_2) / (k_1 - iT) = N\pi / B(K_0 - iT)$$

Equation (2.4.3) is solved by the direct method and yields,

$$f^{(1)}(k_1 k_2) = \frac{\delta(k_1 - K_0) N}{k_2^2 + B^2} - \frac{A}{4\pi^2} \frac{1}{k_2^2 + k_2^2 - E} \quad (2.4.5)$$

$$\cdot \left[\frac{C_B}{k_1 + iT} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} + D_B \left\{ \frac{Bi}{(\sqrt{E - k_1^2} - Bi)(\sqrt{E - k_1^2} + Ti)} + \frac{1}{k_2 + iT} \right\} \right]$$

Its asymptotic part is

$$f^{(1)}(k_1 k_2) \sim \frac{\delta(k_1 - K_0) N}{k_2^2 + B^2} - \frac{A}{4\pi^2} \frac{N\pi}{B} \left[\frac{C_B}{k_1 + iT} + \frac{D_B}{i(B+T)} \right] \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 - K_0^2} \quad (2.4.6)$$

$$- \frac{A}{4\pi^2} \frac{1}{k_1^2 + k_2^2 - E} \left[\frac{C_B}{(k_1 + iT)(|k_2| - Bi)} + D_B \left\{ \frac{Bi}{(|k_2| - Bi)(|k_2| + iT)} + \frac{1}{k_2 + iT} \right\} \right]$$

If this result is compared with the asymptotic part of the exact solution, equation (2.3.2), we see that the form of the solutions is the same. The same formulas for the scattering cross sections can be used with C and D replaced by C_B and D_B . The validity and range of applicability of the Born approximation depends on how well the exact constants C and D are approximated by C_B and D_B . This can be determined by comparing (2.4.4) with (2.2.16). It is clear that for $A \rightarrow 0$ or for those values of E such that the products of A and J_i ($i = 1, 2, 3, 4$) are very much less than 1, that the results obtained from the Born approximation will be useful approximations to the exact results. The J_i are functions of E which approach zero for sufficiently large E so that the products AJ_i can be made small for E sufficiently large. The explicit dependence of J_i on E is given in Appendix I.

These results are well known and represent in detail the motivation for employing the Born approximation. Physically, if the energy of the incident particle is sufficiently large or the interaction between the incident and bound particle extremely small then we expect the initial state of the system to undergo a negligible amount of distortion. Under such conditions the initial state or unperturbed solution should be a good approximation to the exact solution. There is, however, one point that needs further investigation even under these favorable conditions. This is the problem of determining what is meant by the statement that the energy must be sufficiently large for the Born approximation to be good. Jost and Pais³⁸ in an analysis of the Born approximation for a Yukawa potential reached the conclusion that the value of the energy for which the Born approximation gives good results is so large that for all practical purposes the approximation is useless for that potential. A similar analysis was undertaken for equation (2.4.1) and the

38. loc. cit.

results lead to somewhat the same conclusion. Before presenting the numerical results of this work an analysis of the iteration procedure which starts with the unperturbed solution will be found to be illuminating.

The iteration procedure is equivalent to assuming that

$$f(k_1 k_2) = \sum_{n=0}^{\infty} A^n f^{(n)}(k_1 k_2) \quad (2.4.7)$$

This power series in A will be henceforth referred to as the Born expansion. Substituting this series into (2.4.1), and equating the coefficients of like powers of A, we find that for $n = 0$,

$$(k_1^2 + k_2^2 - E) f^{(0)}(k_1 k_2) - (B/\hbar) \int f^{(0)}(k_1 k_2) dk_2 = 0, \quad (2.4.8)$$

and for $n \geq 1$,

$$(k_1^2 + k_2^2 - E) f^{(n)}(k_1 k_2) - (B/\hbar) \int f^{(n)}(k_1 k_2) dk_2 = - \frac{1}{4\pi^2} \left\{ \frac{C_{n-1}}{k_1 + iT} + \frac{D_{n-1}}{k_2 + iT} \right\}, \quad (2.4.9)$$

in which

$$C_{n-1} = \int dk_1 dk_2 f^{(n-1)}(k_1 k_2) / (k_2 - iT)$$

and (2.4.10)

$$D_{n-1} = \int dk_1 dk_2 f^{(n-1)}(k_1 k_2) / (k_1 - iT) .$$

Equation (2.4.8) represents the unperturbed system and its solution is the initial state of the system. Equations (2.4.9) represent the additional contributions to the initial state that arise from the interaction between the particles. Hence the condition which must be placed on $f^{(n)}(k_1 k_2)$, for $n \geq 1$, is that they represent outgoing particles.

Equations (2.4.9) can be solved by the direct method. We find, for $n \geq 1$, that

$$f^{(n)}(k_1 k_2) = - \frac{1}{4\pi^2} \left[\frac{C_{n-1}}{k_1 + iT} \frac{\sqrt{E-k_1^2}}{\sqrt{E-k_1^2} - Bi} + D_{n-1} \left\{ \frac{Bi}{(\sqrt{E-k_1^2} - Bi)(\sqrt{E-k_1^2} + iT)} + \frac{1}{k_2 + iT} \right\} \right] \frac{1}{k_1^2 + k_2^2 - E} \quad (2.4.11)$$

which can be written in matrix notation as

$$f^{(n)}(k_1 k_2) = (h, g) \begin{pmatrix} C_{n-1} \\ D_{n-1} \end{pmatrix}; \quad n \geq 1, \quad (2.4.12)$$

where

$$h \equiv h(k_1 k_2) = - \frac{1}{4\pi^2} \frac{\sqrt{E-k_1^2}}{\sqrt{E-k_1^2} - Bi} \frac{1}{k_1 + iT} \frac{1}{k_1^2 + k_2^2 - E} \quad (2.4.13)$$

$$g \equiv g(k_1 k_2) = - \frac{1}{4\pi^2} \left\{ \frac{Bi}{(\sqrt{E-k_1^2} - Bi)(\sqrt{E-k_1^2} + iT)} + \frac{1}{k_2 + iT} \right\} \frac{1}{k_1^2 + k_2^2 - E}$$

Inserting (2.4.12) into (2.4.10), we obtain

$$C_n = \alpha C_{n-1} + \beta D_{n-1} \quad (2.4.14)$$

$$D_n = \gamma C_{n-1} + \delta D_{n-1}$$

where

$$\alpha = \int dk_1 dk_2 h(k_1 k_2) / (k_2 - iT); \quad \beta = \int dk_1 dk_2 g(k_1 k_2) / (k_2 - iT) \quad (2.4.15)$$

$$\gamma = \int dk_1 dk_2 h(k_1 k_2) / (k_1 - iT); \quad \delta = \int dk_1 dk_2 g(k_1 k_2) / (k_1 - iT).$$

Equation (2.4.14) becomes in matrix notation

$$\begin{pmatrix} C_n \\ D_n \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} C_{n-1} \\ D_{n-1} \end{pmatrix}; \quad n \geq 1, \quad (2.4.16)$$

which gives

$$\begin{pmatrix} C_n \\ D_n \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}^n \begin{pmatrix} C_0 \\ D_0 \end{pmatrix} \quad (2.4.17)$$

Hence equation (2.4.12) becomes

$$f^{(n)}(k_1 k_2) = (h, g) \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}^{n-1} \begin{pmatrix} C_0 \\ D_0 \end{pmatrix} ; \quad n \geq 1. \quad (2.4.18)$$

Substitute (2.4.18) into (2.4.7) and sum. The result is

$$\begin{aligned} f(k_1 k_2) = f_0(k_1 k_2) + A m \left\{ \left[(1 - A\delta) C_0 + A\beta D_0 \right] h(k_1 k_2) \right. \\ \left. + \left[A\gamma C_0 + (1 - A\alpha) D_0 \right] g(k_1 k_2) \right\} \end{aligned} \quad (2.4.19)$$

with the determinant

$$m^{-1} = \begin{vmatrix} 1 - A\alpha & -A\beta \\ -A\gamma & 1 - A\delta \end{vmatrix},$$

and

$$C_0 = \int dk_1 dk_2 f_0(k_1 k_2) / (k_2 - iT) = N\pi i / B(B + T) = C_B, \quad (2.4.20)$$

$$D_0 = \int dk_1 dk_2 f_0(k_1 k_2) / (k_1 - iT) = N\pi / B(K_0 - iT) = D_B.$$

From equation (2.4.8) it is evident that $f^{(0)}(k_1 k_2)$ is equal to $f_0(k_1 k_2)$.

The evaluation of the integrals in (2.4.15) gives

$$\alpha = \delta = iJ_1 / 4\pi ; \quad \gamma = J_4 / 4\pi T \quad (2.4.21)$$

$$\beta = - (BJ_2 + iJ_3) / 4\pi ,$$

where $J_i (i = 1, 2, 3, 4)$ are the same quantities which occur in (2.2.16).

Combining equations (2.4.19), (2.4.20) and (2.4.21) we obtain the exact

solution given by equation (2.2.18). From (2.4.21) it follows that $m = \Delta$,

the latter quantity appearing in equation (2.2.17).

The series solution obtained by the iteration procedure converges to the exact solution. The series itself represents the exact solution only for those values of the parameters which lie within the radius of convergence of the series. In practice, where only a few terms in the Born expansion can be evaluated, the domain of applicability or validity of the resulting approximation is restricted by the radius of convergence of this series representation. The radius of convergence of the Born expansion, ρ , taken for convenience to be expressed as $|A/4\pi|$, is given by the smaller in absolute value of the two roots for $A/4\pi$ of

$$\Delta^{-1} = m^{-1} = (1 - \frac{A}{4\pi} J_1 i)^2 + \left(\frac{A}{4\pi}\right)^2 \frac{J_4}{T} (BJ_2 + iJ_3) = 0. \quad (2.4.22)$$

The graph, Figure 1, is a plot of the radius of convergence ρ as a function of the energy in units of B^2 i.e., $Z = E/B^2$. To obtain the curve, T was set equal to $2B$. The interpretation of the curve is as follows: For a given Z_1 , the series converges for all values of $|A/4\pi| < \rho_1$ where ρ_1 is the value associated with Z_1 , by the curve. Of if ρ_1 is given and Z_1 is associated with this value, then for all $Z > Z_1$, the series solution converges. It follows that for a given $A/4\pi$ the best that can be expected from the series representation is the value of the exact solution for all $Z > Z_1$ where Z_1 is the energy associated with the absolute value of the given $A/4\pi$. For $Z < Z_1$, the series representation diverges. For large values of the total energy E the radius of convergence approximates

$$\rho \sim T(E)^{1/2} / \pi = BT(Z)^{1/2} / \pi \quad (2.4.23)$$

This means that in this region for the total energy a small change in A requires a very large change in the value for E for which the series would still converge.

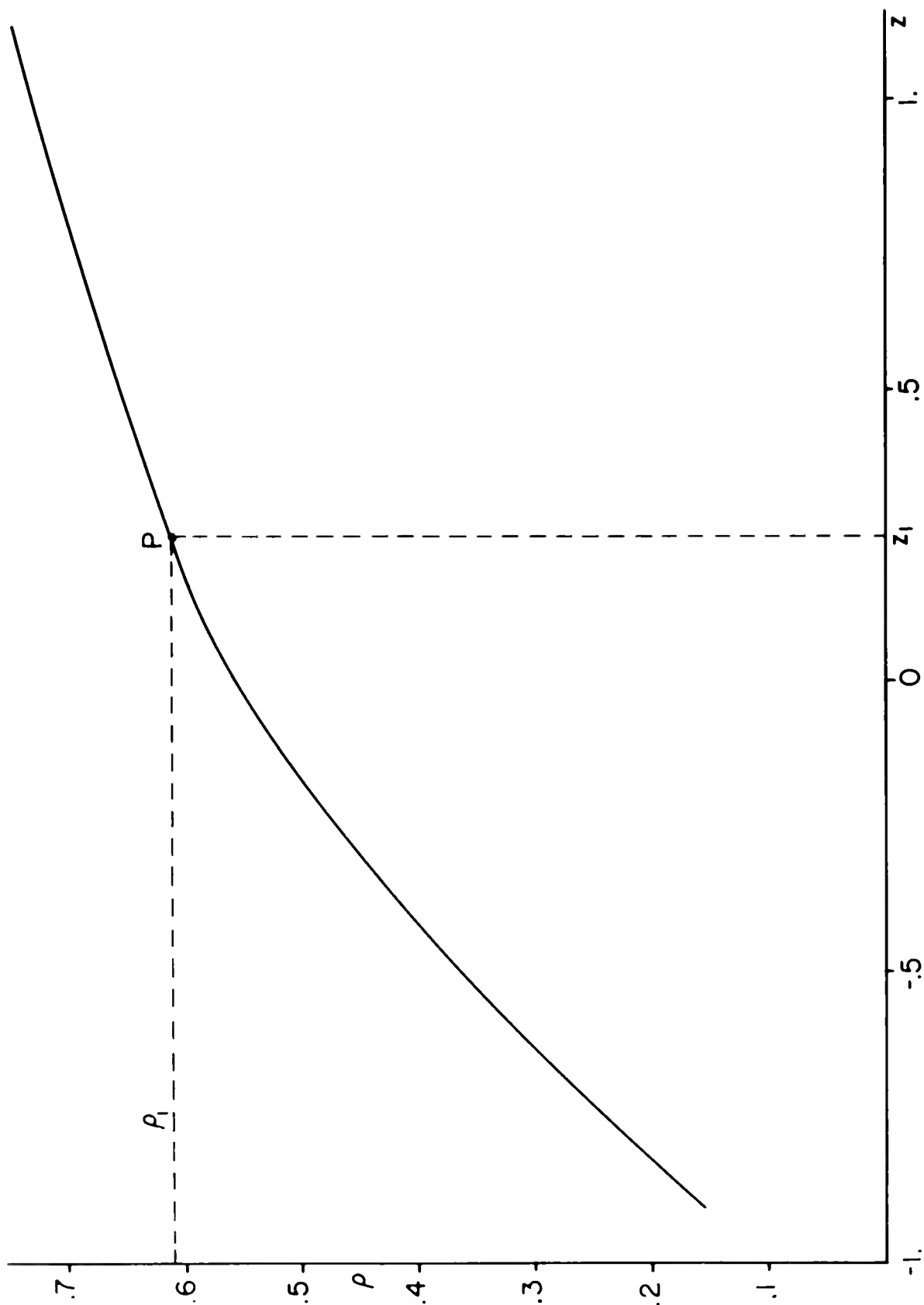


Figure 1

The Born approximation is obtained from the series expansion (2.4.7) if $f^{(n)}(k_1 k_2)$ is set equal to zero for all $n \geq 2$. The series is then represented by its first two terms. This approximation should be good for "energies sufficiently large." Using the expressions obtained in Appendix I for J_i ($i = 1, 2, 3, 4$) for large values of E , in the exact formulas for C and D , we find that C is approximated very well by C_B but that D does not approach D_B unless

$$A/4\pi \ll T(B+T)/\pi \quad (2.4.24)$$

The constant B is related to the bound state energy whereas the constant T is related to the range of the interaction in its space coordinate representation. Note that both relations (2.4.23) and (2.4.24) depend on the range of the interaction. Equation (2.4.23) assures the existence of a radius of convergence for the Born expansion no matter how small T is taken, i.e., for long range interactions, if the total energy E is taken sufficiently large, say, $E \sim kT^{-2}$ with k constant. However (2.4.24) asserts that no matter how large E is taken if this relation is not satisfied then the Born approximation has no range of validity. For the Born approximation to yield useful results two conditions must be met: first, the energy must be large and secondly the interaction must be weak. By weak we mean the satisfaction of equation (2.4.24).

The scattering cross sections (2.3.9) and (2.3.10) for large values of E become

$$Q_i = A^2 |C|^2 / 8\pi TE \quad (2.4.25)$$

and

$$Q_e = (A^2 B / 4\pi E) \left[\frac{|C|^2}{E} + \frac{|D|^2}{(B+T)^2} \right] \quad (2.4.26)$$

Since the exact C approaches the Born value C_B , the inelastic scattering cross sections for these solutions will be in good agreement for large values of the energy. However, unless (2.4.24) is satisfied, D does not approach D_B . The exact and Born calculation for the elastic scattering cross section can not possibly approach each other no matter how large E is taken.

Next consider the second Born approximation which we define as the first three terms in the Born expansion. For large values of the total energy E the constants C and D are approximated by the expressions C_{2B} and D_{2B} which are given by

$$C_{2B} = C_B \quad (2.4.27)$$

and

$$D_{2B} = D_B \left\{ 1 + \frac{A}{4\pi} \frac{\pi}{T(B+T)} \right\} \quad (2.4.28)$$

These values are precisely the values for C and D for large values of E .

Thus the scattering cross sections calculated for the second Born approximation will agree with the exact values if E is sufficiently large. Furthermore equations (2.4.27) and (2.4.28) are not restricted by any condition on the magnitude of A . This is a distinct improvement over the Born approximation. As a matter of fact the ratio of the elastic scattering cross sections calculated from the second Born approximation to that calculated from the Born approximation is

$$\frac{1}{2} \left\{ 1 + \left(1 + \frac{A}{4\pi} \frac{\pi}{T(B+T)} \right)^2 \right\} \quad (2.4.29)$$

for large values of E . This ratio is a constant and it indicates that in general the second Born approximation is a substantial correction to the Born approximation.

The significance of the second Born approximation resides in the fact that it takes into account the second and third terms in the Born expansion.

These two terms are the leading terms in a power series expansion for the outgoing scattered wave. Their ratio can be used as a measure of the rapidity of the convergence of the series. This ratio also expresses the pertinent physical aspect of the problem. The first term in the Born expansion represents the initial state of the system and is independent of the interaction between the particles. It is the second term in the expansion which first exhibits the effects of the interaction on the initial state. Hence to get some idea of the total effect of this interaction, the third and second terms of the expansion must be compared. A similar point will arise when Born type trial functions are used in the Schwinger variational principle.

The problem treated by Jost and Pais led to results similar in content to equations (2.4.24) and (2.4.29). Furthermore Dalitz evaluated terms in the Born expansion of the problem he considered up to and including the third order terms. The terms to the second order are sufficient to indicate the convergence of the expansion for the wave function. Hence the above results are not peculiar to the specific problem studied.

Table I contains the exact values for the elastic, Q_e , and inelastic, Q_i , scattering cross sections for various values of the total energy E with the parameters $A/4\pi$ set equal to 1 and T equal to $2B$. For these same values of the parameter the radius of convergence, ρ , has been tabulated as well as the elastic, Q_{eB} , and inelastic, Q_{iB} , scattering cross sections calculated from the Born approximation. The Born results are unsatisfactory for $\rho < 1$. The general discussion of the Born expansion would lead us to expect this result. For $\rho > 1$ Q_{iB} improves steadily while Q_{eB} fails to approach the exact Q_e even for large values of the energy. These results are confirmations of the discussion given above.

The preceding work indicates that in general to obtain useful results

higher order terms in the Born expansion must be calculated. In practice this is very difficult to do, so that other methods must be used. Among these are the variational procedures and in particular the Hulthén-Kohn and Schwinger variational principles which will now be considered.

2.5 Hulthén-Kohn Variational Principle

Equation (2.1.3) with the interaction given by (2.1.5) is reconsidered. For convenience these equations are again written down.

(2.5.1)

$$(k_1^2 + k_2^2 - E)f(k_1 k_2) - (B/\pi) \int f(k_1 k_2) dk_2 + (1/4\pi^2) \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f(k_1' k_2') = 0$$

and

$$(k_1 k_2 | V | k_1' k_2') \equiv A \left\{ -\frac{1}{(k_1 + iT)(k_2' - iT)} + \frac{1}{(k_2 + iT)(k_1' - iT)} \right\} \quad (2.5.2)$$

In terms of the Green's function, equation (2.5.1) can be represented by the following integral equation,

(2.5.3)

$$f(k_1 k_2) = f_0(k_1 k_2) - (1/4\pi^2) \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2''),$$

where $f_0(k_1 k_2)$ is a solution of the unperturbed Schroedinger equation and

represents the initial state of the system. The Green's function

$G(k_1 k_2; k_1' k_2')$ is given by equation (2.2.37) or (2.2.38). With this function

(2.5.1) can be written

$$f(k_1 k_2) = f_0(k_1 k_2) + \int \frac{(K_1 k_2 | k_1 k_2) dK_1 f(K_1)}{K_1^2 - K_0^2} + \int \frac{(K_1 k_2 | k_1 k_2) dK_1 dK_2 f(K_1 K_2)}{K_1^2 + K_2^2 - E} \quad (2.5.4)$$

with $K_0^2 = B^2 + E$ and

Table I

z	Exact		Radius of Convergence	Born	
	Q_e	Q_i	ρ	Q_{eB}	Q_{iB}
-9	1.981103		.153299	84.3468	
-5	1.855550		.363870	14.72996	
-1	1.655647		.518062	7.22660	
-.05	1.622907		.536320	6.74632	
-.01	1.592725		.550914	6.39884	
-.005	1.588288		.552750	6.35748	
-.001	1.584349		.554227	6.32468	
+.001	1.581312	.000476	.554833	6.30840	.0016854
+.005	1.574897	.002350	.555733	6.27604	.00842896
+.01	1.567423	.004652	.556832	6.23596	.0167470
+.05	1.515046	.022342	.565409	5.93000	.0789516
.1	1.458419	.042524	.57573	5.58064	.147110
.5	1.150270	.152834	.65061	3.67353	.451456
.9	.962272	.210601	.71706	2.62637	.549148
5.	.338524	.236493	1.23844	.409404	.356102
10.	.154223	.165691	1.73059	.134696	.205592
100.	.002788	.021490	6.10792	.001718	.020981
1000.	.000029	.002190	20.03332	.000018	.002192

$z = E/B^2$, E is the total energy.

Q_e = exact elastic scattering cross section.

Q_i = exact inelastic scattering cross section.

Q_{eB} = Born elastic scattering cross section.

Q_{iB} = Born inelastic scattering cross section.

ρ = radius of convergence of the Born expansion in units of B^2 .

$$f(K_1) = -(1/4\pi^2) \int (K_1^2 |k_1' k_2')^* dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2''), \quad (2.5.5)$$

$$f(K_1 K_2) = - (1/4\pi^2) \int (K_1 K_2 | k_1' k_2')^* dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2'').$$

Associated with the integral equation (2.5.3) is an adjoint integral equation which represents solutions of equation (2.5.1) expressed in terms of incident waves plus incoming or concentrating waves. The Green's function for these solutions will be indicated by a subscript c. The relationship between the Green's functions is

$$G_c(k_1 k_2; k_1' k_2') = G^*(k_1' k_2'; k_1 k_2) \quad (2.5.6)$$

The integral equation representation of these solutions is

$$(2.5.7)$$

$$f_1(k_1 k_2) = f_{01}(k_1 k_2) - (1/4\pi^2) \int G_c(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f_1(k_1'' k_2'')$$

where $f_{01}(k_1 k_2)$ is a solution of the unperturbed Schroedinger equation.

The specific solution desired will be indicated later. This equation becomes

$$f_1(k_1 k_2) = f_{01}(k_1 k_2) - (1/4\pi^2) \int f_1(k_1'' k_2'') dk_1'' dk_2'' (k_1'' k_2'' | V | k_1' k_2')^* dk_1' dk_2' G^*(k_1' k_2'; k_1 k_2) \quad (2.5.8)$$

when use is made of the hermitian property of the interaction and the relation (2.5.6).

The Hulthén-Kohn variational principle³⁹ is based upon the consideration of the following functional,

$$I_1 = I \left\{ v_1, v \right\} = \lim_{E' \rightarrow E} \int v_1^* (k_1 k_2; E') \left\{ H - E \right\} v(k_1 k_2; E) dk_1 dk_2, \quad (2.5.9)$$

39. H. E. Moses, Phys. Rev. 92, 817 (1953).

in which

$$\begin{aligned} \{H - E\} v(k_1 k_2; E) &\equiv (k_1^2 + k_2^2 - E) v(k_1 k_2; E) - (B/\pi) \int v(k_1 k_2; E) dk_2 \\ &+ (1/4\pi^2) \int (k_1 k_2 | V | k_1^! k_2^!) dk_1^! dk_2^! v(k_1^! k_2^!; E). \end{aligned} \quad (2.5.10)$$

The functions $v(k_1 k_2; E)$ and $v_i(k_1 k_2; E)$ are arbitrary. The limiting process indicated in (2.5.9) is to be executed after the integrations have been performed. This is necessary for the $v(k_1 k_2; E)$ and $v(k_1 k_2; E')$ are singular and to treat the singularities in a consistent manner (see footnote 39) the above limiting procedure must be used.

Equation (2.5.9) will be varied about those solutions of

$$\{H - E\} f(k_1 k_2; E) = 0, \quad (2.5.11)$$

and

$$\{H - E'\} f_i(k_1 k_2; E') = 0, \quad (2.5.12)$$

which are represented by the integral equations (2.5.3) and (2.5.8) respectively. The variation of (2.5.9) about these solutions yields

$$\delta I_i = \lim_{E' \rightarrow E} \int \delta f(k_1 k_2; E) \{E' - E\} f_i^*(k_1 k_2; E') dk_1 dk_2. \quad (2.5.13)$$

The variations about the solutions of (2.5.11) and (2.5.12) are now restricted to have the following form

$$\delta f(k_1 k_2; E) = \int \frac{(K_1 K_2 | k_1 k_2) dK_1 \delta f(K_1)}{K_1^2 - K_0^2} + \int \frac{(K_1 K_2 | k_1 k_2) dK_1 dK_2 \delta f(K_1 K_2)}{K_1^2 + K_2^2 - E}$$

Variations of this type require that the inhomogeneous term of the correct solution is to be unaltered. These variations have the further property of admitting trial functions which differ from the exact solution only in the amplitudes of the scattered waves. Substitute (2.5.14) into (2.5.13)

choose f_{o1} so that $f_{o1} = (K_1^2 | k_1 k_2)$ with $K_1^2 = B^2 + E$ and $f_{o2} = (K_1 K_2 | k_1 k_2)$ with $K_1^2 + K_2^2 = E$. Then we find that

$$\delta(I_1 - f(K_o)) = 0 ; \quad K_o^2 = B^2 + E \quad (2.5.15)$$

and

$$\delta(I_2 - f(K_1 K_2)) = 0 ; \quad K_1^2 + K_2^2 = E \quad (2.5.16)$$

These equations assert that trial functions, which we denote by a subscript t , which differ from the exact functions in the first order determine $f(K_o)$ and $f(K_1 K_2)$, ($K_1^2 + K_2^2 = E$) correctly to the first order. Thus, for trial functions, equations (2.5.15) and (2.5.16) take the form,

$$I_{1t} - f_t(K_o) = -f(K_o); \quad K_o^2 = B^2 + E \quad (2.5.17)$$

and

$$I_{2t} - f_t(K_1 K_2) = -f(K_1 K_2); \quad K_1^2 + K_2^2 = E$$

It should be noticed that these equations determine approximations to $f(K_1)$ and $f(K_1 K_2)$ only in a restricted domain of their arguments. But the values so determined are just those needed to obtain the asymptotic part of the wave function. Equations (2.5.17) determine the functions at the singularities which occur in the integrands of equation (2.5.4).

One disadvantage of this variational principle is apparent. Since $f(K_1)$ and $f(K_1 K_2)$ are known approximately only for a restricted domain of their arguments, an iterative procedure to improve the trial functions by substituting the variational results into equation (2.5.4) would not be satisfactory. The amplitudes of the scattered waves depend on the interaction of the particles when they are close to each other and this means that $f(K_1)$ and $f(K_1 K_2)$ should be approximately known throughout the range of values of their respective arguments. This knowledge is not forthcoming from the variational principle.

The mathematical simplicity of the Hulthén-Kohn variational principle makes it feasible to employ a very large class of trial functions. However, we shall be interested in comparing the results with those obtained from the Born approximation and from the Schwinger variational principle. The trial functions are therefore restricted to be of the Born type, i.e., the solutions of the unperturbed equation. For such trial functions the Hulthén-Kohn variational principle can readily be shown to give the same results as the Born approximation. This follows immediately from equations (2.5.17) when compared with (2.5.4) and (2.5.5). For our purposes the Hulthén-Kohn procedure is the equivalent of the Born approximation. However, in the following discussion of the Schwinger variational principle we shall note certain similarities between these principles which will be further explored in the succeeding section.

2.6 The Schwinger Variational Principle

The integral equations (2.5.3) and (2.5.8) are rewritten in the following way,

(2.6.1)

$$f_o(k_1 k_2) = f(k_1 k_2) + (1/4\pi^2) \int G(k_1 k_2; k_1''' k_2''') dk_1'' dk_2'' (k_1''' k_2''' | V | k_1'' k_2'') \cdot dk_1'' dk_2'' f(k_1'' k_2''),$$

and

(2.6.2)

$$f_{oi}(k_1 k_2) = f_i(k_1 k_2) + (1/4\pi^2) \int f_i(k_1'' k_2'') dk_1'' dk_2'' (k_1'' k_2'' | V | k_1''' k_2''')^* \cdot dk_1''' dk_2''' G^*(k_1''' k_2'''; k_1 k_2).$$

Multiply these equations with $(k_1' k_2' | V | k_1 k_2) dk_1 dk_2$ and integrate over the indicated variables. The resulting equations can then be written in the forms

$$a(k_1 k_2) = K f(k_1' k_2') \quad (2.6.3)$$

and

$$e_i(k_1 k_2) = K' f_i(k_1' k_2') \quad (2.6.4)$$

where

$$a(k_1 k_2) = \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f_0(k_1' k_2'), \quad (2.6.5)$$

$$a_1(k_1 k_2) = \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f_{01}(k_1' k_2'), \quad (2.6.6)$$

and K, K' are integral operators with kernels

$$(2.6.7)$$

$$K(k_1 k_2; k_1' k_2') = \int \left[\delta(k_1 - k_1'') \delta(k_2 - k_2'') + (1/4\pi^2) (k_1 k_2 | V | k_1'' k_2'') dk_1'' dk_2'' G(k_1'' k_2''; k_1' k_2') \right] \\ \cdot dk_1'' dk_2'' (k_1'' k_2'' | V | k_1' k_2'),$$

and

$$(2.6.8)$$

$$K'(k_1 k_2; k_1' k_2') = \int (k_1' k_2' | V | k_1'' k_2'')^* dk_1'' dk_2'' \left[\delta(k_1 - k_1'') \delta(k_2 - k_2'') \right. \\ \left. + (1/4\pi^2) G^*(k_1'' k_2''; k_1'' k_2'') dk_1'' dk_2'' (k_1'' k_2'' | V | k_1 k_2)^* \right]$$

respectively. The meaning of equation (2.6.3) is that

$$a(k_1 k_2) = \int K(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2')$$

with a similar interpretation for equation (2.6.4). From (2.6.7) and

(2.6.8) it follows that

$$K'(k_1 k_2; k_1' k_2') = K^*(k_1' k_2'; k_1 k_2) \quad (2.6.9)$$

which asserts that K' is the hermitian adjoint of K . From (2.6.3), (2.6.4)

and (2.6.9) we obtain

$$(f_1, a) = (f_1, Kf) = (K'f_1, f) = (a_1, f), \quad (2.6.10)$$

in which the expression (x, y) represents the hermitian inner product of the quantities embraced. The dependence of the quantities in (2.6.10) on the variables k_1, k_2 has been omitted for the sake of brevity and simplicity.

The Schwinger variational principle (see footnotes 7,8) states that the expression

$$\lambda \left\{ v_1, v \right\} = (v_1, Kv) / (v_1, a)(a_1, v) \quad (2.6.11)$$

is stationary for independent variations of the arbitrary functions v and v_1 about the solutions f and f_1 of the integral equations (2.6.1) and (2.6.2). For $v = f$ and $v_1 = f_1$

$$\lambda = \lambda \{f_1, f\} = 1/(a_1, f) = 1/(f_1, a). \quad (2.6.12)$$

Note that for $v = f$ and v_1 arbitrary

$$\lambda \{v_1, f\} = 1/(a_1, f). \quad (2.6.13)$$

The stationary property of (2.6.11) serves as a variational calculation for $1/(a_1, f)$ or $1/(f_1, a)$. The term

$$(a_1, f) = \int f_{oi}^*(k_1 k_2) dk_1 dk_2 (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f(k_1' k_2'), \quad (2.6.14)$$

corresponds to $f(K_1)$ or $f(K_1 K_2)$ of (2.5.5) provided that $f_{oi}(k_1 k_2)$ can be replaced by $(K_1 2 | k_1 k_2)$ or $(K_1 K_2 | k_1 k_2)$ respectively. However, $f_{oi}(k_1 k_2)$ must be a solution of the unperturbed wave equation whereas $(K_1 2 | k_1 k_2)$ and $(K_1 K_2 | k_1 k_2)$ are not solutions unless $K_1^2 = K_0^2 = B^2 + E$ for the former and $K_1^2 + K_2^2 = E$ for the latter. If these functions are used, with the values of their arguments so restricted, in place of $f_{oi}(k_1 k_2)$ in (2.6.14), then $-(a_1, f)/4\pi^2$ takes on the values $f(K_0)$ and $f(K_1 K_2)$, which are the values of the exact functions at the singularities of the integrands of (2.5.4). Exactly the same result was obtained in the discussion of the Hulthén-Kohn variational principle. Hence the Schwinger variational principle yields approximations to the amplitudes of the scattered waves only.

The exact expressions (2.6.14) are equal to

$$(a_i, f) = A \left[CP_{1i} + DP_{2i} \right], \quad i = 1, 2 \quad (2.6.15)$$

where

$$P_{11} = \int dk_1 dk_2 (K_1 Z | k_1 k_2)^* / (k_1 + iT) ; \quad P_{12} = \int dk_1 dk_2 (K_1 K_2 | k_1 k_2)^* / (k_1 + iT) \quad (2.6.16)$$

$$P_{21} = \int dk_1 dk_2 (K_1 Z | k_1 k_2)^* / (k_2 + iT) ; \quad P_{22} = \int dk_1 dk_2 (K_1 K_2 | k_1 k_2)^* / (k_2 + iT)$$

The left hand side of equation (2.6.15) is approximated by the Schwinger variational principle. This equation then yields the approximate values for the constants C and D. In this way we obtain the exact solution except for the values of the constants C and D. The approximate values for C and D may be inserted in the formulas for the scattering cross section to obtain the variational results.

Before discussing the results obtained from the Schwinger variational principle when Born trial functions are used, it is worthwhile to consider the expression for $\lambda \{v_1, v\}$ in detail.

Let P and Q be two integral operators with kernels $1/(k_1 - iT)$ and $1/(k_2 - iT)$ respectively. Then for any function $f(k_1 k_2)$,

$$P(f) \equiv \int dk_1 dk_2 f(k_1 k_2) / (k_1 - iT) \quad (2.6.17)$$

and

$$Q(f) \equiv \int dk_1 dk_2 f(k_1 k_2) / (k_2 - iT) . \quad (2.6.18)$$

Then

$$\begin{aligned} (v_1, Kv) = A \left[P^*(v_1)Q(v) + Q^*(v_1)P(v) \right] \\ + (A^2/4\pi) \left[(-iJ_1)(P^*(v_1)Q(v) + Q^*(v_1)P(v)) \right. \\ \left. + (BJ_2 + iJ_3)P^*(v_1)P(v) - (J_4/T)Q^*(v_1)Q(v) \right], \end{aligned} \quad (2.6.19)$$

where J_i ($i = 1, 2, 3, 4$) are defined in equation (2.2.16),

$$(v_1, a) = A \left[P^*(v_1)Q(a) + Q^*(v_1)P(a) \right], \quad (2.6.20)$$

and

$$(a_1, v) = A \left[P^*(a_1)Q(v) + Q^*(a_1)P(v) \right]. \quad (2.6.21)$$

If we assume that the trial function v is symmetric or antisymmetric, then

$$P(v) = \pm Q(v). \quad (2.6.22)$$

The plus sign is to be associated with a symmetric v and the minus sign with an antisymmetric v . This convention will be adhered to in what follows. From equations (2.6.19), (2.6.20), (2.6.21), (2.6.22) and (2.6.11), we find that,

$$\lambda \left\{ v_1, v \right\} = \frac{2+(A/4\pi) \left[-2iJ_1 \pm (BJ_2 + iJ_3) \pm (-J_4/T) \right]}{A \left[Q(a) \pm P(a) \right] \left[P^*(a_1) \pm Q^*(a_1) \right]} \quad (2.6.23)$$

Here the Schwinger variational principle is independent of trial functions which are symmetric or antisymmetric.

The physical problem that is being considered here cannot have either a symmetric or antisymmetric solution because as formulated particle 1 does not interact with the center of force but particle 2 does. For this reason the results obtained from (2.6.23) would be expected to yield very poor approximations to the scattering cross sections. Certainly these trial functions are not "close" to the exact wave function for which case we would expect to get good results from the variational calculations. However, the numerical calculations given in Table III obtained by using symmetric trial functions give surprisingly good results. This indicates that some criterion other than "closeness" is necessary to determine the appropriateness of a given trial function.

Next consider the principle when Born type trial functions are used.

Then

$$\lambda \left\{ f_{01}, f_0 \right\} = (f_{01}, Kf_0) / (f_{01}, a)^2,$$

which becomes, when (2.6.7) is used,

$$= \left[(f_{01}, Vf_0) + (f_{01}, VGVf_0) \right] / (f_{01}, Vf_0)^2 \quad (2.6.24)$$

where

$$Vf_0 \equiv \int (k_1 k_2 |V| k_1' k_2') dk_1' dk_2' f_0(k_1' k_2') = a(k_1 k_2)$$

and

$$VGVf_0 \equiv (1/4\pi^2) \int (k_1 k_2 |V| k_1'' k_2'') dk_1'' dk_2'' G(k_1'' k_2''; k_1' k_2') dk_1' dk_2' f_0(k_1' k_2').$$

From (2.6.24),

$$\begin{aligned} 1/\lambda \{f_{01}, f\} &= (f_{01}, Vf_0 - VGVf_0) + \dots \\ &= (a_1, f_0 - GVf_0) + \dots, \end{aligned} \quad (2.6.25)$$

where equation (2.6.6) has been used to obtain the last equation. Now $f_0 - GVf_0$ is the Born approximation to the exact wave function f . Equation (2.6.25) shows (see footnotes 7, 15) that the Schwinger variational procedure contains the second Born approximation to the scattering amplitude. Since the expansion which led to (2.6.25) implies the existence of a radius of convergence, it would appear that the Schwinger variational procedure which is not so restricted contains more useful information than the Born approximation. However (2.6.25) is valid only if

$$\left| (f_{01}, VGVf_0) / (f_{01}, Vf_0) \right| < 1 \quad (2.6.26)$$

This ratio is nothing else but the ratio of the asymptotic values of the third to second terms in the Born expansion and we have been in section (2.4) that this ratio need not satisfy (2.6.26). Therefore unless the same rather severe restrictions of that section are satisfied, the comparison between the Schwinger variational results and the Born results cannot be made. The expected second Born approximation which we know to be useful is not obtainable from the Schwinger variational principle.

In Appendix II, the expressions for C and D obtained from the Schwinger

variational principle are given. For A small and E large the Schwinger results are the same as the Born results which are adequate under the stated conditions. But for A of reasonable magnitude we found, in section (2.4), that this approximation had no range of applicability. In Appendix II we display several Born type trial functions which, for large values of the energy, make the variational result reduce to the Born result. By stating that several Born type trial functions were used we mean that for a specific energy E the relation $K_1^2 + K_2^2 = E$, which must be satisfied by K_1 and K_2 in $(K_1 K_2 | k_1 k_2) \equiv f_{02}$ of (2.6.2), permits some leeway in the choice of K_1 or K_2 . Thus there are two parameters that may be varied, E and K_1 , say, in the determination of the constants C and D .

Table II represents the results of numerical calculations for two such Born type trial functions. The third and fourth columns represent results from one of the trial functions which are very good for small values of the energy but are poor for very large values of the energy. The results listed in the first two columns are obviously unsatisfactory. The interesting feature of these trial functions is that neither one yields results which approach either the exact or the Born results (Table I) for large values of the energy, which means that (2.6.26) is not satisfied, yet one of the trial functions yields excellent results for small values of E for which the Born approximation is unreliable.

Table III contains the results of the numerical calculations for those trial functions (symmetric or antisymmetric) for which the Schwinger variational principle gave results independent of any of them. The symmetric trial functions give surprisingly good results for small values of the energy. Among these functions are of course the symmetrized Born type trial functions.

The above results emphasize the complexity of the problem of choosing suitable trial functions for the Schwinger variational principle. Though for two body problems (see footnotes 7, 15) equation (2.6.25) seems to be satisfactory, we have seen that this is not necessarily the case for three body problems.

In developing the methods of the last two sections, we noted certain features that were common to the Hulthén-Kohn and Schwinger variational principles. We now turn to a closer examination of both methods.

TABLE II
SCHWINGER VARIATIONAL PRINCIPLE

z	Q_{e1}	Q_{i1}	Q_{e2}	Q_{i2}
- .9	78.0543		1.99102	
- .5	7.82721		1.87292	
- .1	7.76282		1.64441	
- .05	7.74562		1.60664	
- .01	7.72238		1.57217	
- .005	7.71808		1.56716	
- .001	7.71661		1.56271	
+ .001	7.70745	35.0382	1.55937	.000420
+ .005	7.69002	34.7296	1.55236	.002095
+ .010	7.66928	34.7536	1.54415	.004165
+ .050	7.51826	34.9560	1.48623	.019870
+ .1	7.34926	35.2473	1.42358	.037670
+ .5	6.40765	38.1054	1.07304	.131780
+ .9	4.66525	40.6805	.857346	.178022
+ 5.	1.02642	9.40526	.212231	.166743
+ 10.	.384106	12.7160	.075576	.094603
+ 100.	.000089	.230986	.000292	.002346
+ 1000.	.000000	.322939	.000000	.000064

z = ratio of total energy to energy of bound state.

Q_{e1} = elastic cross section for first trial function.

Q_{e2} = elastic cross section for second trial function.

Q_{i1} = inelastic cross section for first trial function.

Q_{i2} = inelastic cross section for second trial function.

$$(A/4\pi = 1)$$

TABLE III

z	Symmetric Solution		Antisymmetric Solution	
	σ_{es}	σ_{is}	σ_{ea}	σ_{ia}
-.9	1.98668		.399036	
-.5	1.89174		.143718	
-.1	1.71993		.114093	
-.05	1.67722		.112869	
-.01	1.64642		.112441	
-.005	1.64182		.112470	
-.001	1.63771		.112540	
+.001	1.63449	.000440	.112611	.0000788
.005	1.62749	.002196	.112649	.0003950
.01	1.61934	.004370	.112622	.0007906
.05	1.56166	.020896	.111948	.0039010
.1	1.49869	.039700	.110622	.0076240
.5	1.14633	.141436	.0979432	.0314150
.9	.927302	.194124	.0867578	.0465544
5.	.259336	.211024	.0374990	.0641592
10.	.107261	.135296	.0215910	.0490688
100.	.00349740	.0101514	.00241656	.00799950
1000.	.000254130	.0008708	.0002436	.00084758

z = total energy in units of Bound state energy (E/B^2).

σ_{es} = elastic scattering cross section determined by symmetric trial functions.

σ_{is} = inelastic scattering cross section determined by symmetric trial functions.

σ_{ea} = elastic scattering cross section determined by antisymmetric trial functions.

σ_{ia} = inelastic scattering cross section determined by antisymmetric trial functions.

2.7 Relation between the Hulthén-Kohn and Schwinger Variational Principles

The Hulthén-Kohn variational principle is based on the functional

$$I \{v_i, v\} = \lim_{E' \rightarrow E} \int v_i^*(k_1 k_2; E') \{H - E\} v(k_1 k_2; E) dk_1 dk_2. \quad (2.7.1)$$

The notation employed here and the significance of equation (2.7.1) has been explained in section (2.5). Let

$$v(k_1 k_2; E) = f_0(k_1 k_2) - [(f_{01}, Vf) / (f_{01}, Vg)] Gv_g, \quad (2.7.2)$$

in which

$$Vh \equiv (1/4\pi^2) \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' h(k_1' k_2')$$

and

$$GVh \equiv (1/4\pi^2) \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' h(k_1'' k_2''),$$

for any function $h(k_1 k_2)$. The function $g(k_1 k_2)$ is arbitrary but the functions f_0 , f_{01} and f are those defined in section (2.5). For g set equal to f in (2.7.2) v becomes equal to f so that (2.7.2) can be considered as an admissible trial function for the Hulthén-Kohn variational principle.

The Hulthén-Kohn variational principle gave the following relations,

$$\delta I_1 = \delta f(K_0); K_0^2 = B^2 + E, \quad (2.7.4)$$

and

$$\delta I_2 = \delta f(K_1 K_2); K_1^2 + K_2^2 = E \quad (2.7.5)$$

where $f(K_0)$ and $f(K_1 K_2)$ are the asymptotic parts of $f(K_1)$ and $f(K_1 K_2)$ defined by (2.5.5). These asymptotic parts can be expressed as follows,

$$f(K_0) = - (f_{01}, Vf); K_0^2 = B^2 + E \quad (2.7.6)$$

and

$$f(K_1 K_2) = - (f_{02}, Vf); K_1^2 + K_2^2 = E. \quad (2.7.7)$$

The corresponding asymptotic parts of (2.7.2) are

$$(2.7.8)$$

$$v(K_0) = - [(f_{01}, Vf) / (f_{01}, Vg)] (f_{01}, Vg) = - (f_{01}, Vf); K_0^2 = B^2 + E$$

and similarly

$$v(K_1 K_2) = - (f_{02}, Vf); \quad K_1^2 + K_2^2 = E. \quad (2.7.9)$$

These are exactly the same as (2.7.6) and (2.7.7) respectively. It follows that for such trial functions $v(k_1 k_2; E)$ that equations (2.7.4) and (2.7.5) reduce to

$$\delta I_i = 0, \quad (i = 1, 2). \quad (2.7.10)$$

In other words equation (2.7.2) defines trial functions which have exactly the same asymptotic parts as the exact wave function.

Now evaluate (2.7.1) by substituting (2.7.2) for v . Then

$$I\{v_1, v\} = I\{v_1, \varepsilon\} = (v_1, Vf_0) - \left\{ (f_{01}, Vf) / (f_{01}, v\varepsilon) \right\} \left\{ (v_1, v\varepsilon) + (v_1, vGV\varepsilon) \right\}. \quad (2.7.11)$$

The term in curly brackets may be written $(v_1, K\varepsilon)$ where K is the integral operator defined by (2.6.7). Then (2.7.11) becomes

$$I\{v_1, \varepsilon\} = (v_1, Vf_0) - (f_{01}, Vf)(v_1, Vf_0) \lambda\{v_1, K\varepsilon\} \quad (2.7.12)$$

in which

$$\lambda\{v_1, K\varepsilon\} = (v_1, K\varepsilon) / (v_1, Vf_0)(Vf_{01}, \varepsilon).$$

$\lambda\{v_1, K\varepsilon\}$ is the quantity in terms of which the Schwinger variational principle is formulated.

Consider the variation of the functional $I\{v_1, v\}$ about the exact solutions f_1 and f . This is equivalent to varying v_1 and ε independently about the exact solutions. We find that

$$\delta I \left\{ v_1, v \right\}_{\substack{v = f \\ v_1 = f_1}} = -(f_{01}, Vf)^2 \delta \lambda \left\{ v_1, K\varepsilon \right\}_{\substack{\varepsilon = f \\ v_1 = f_1}}. \quad (2.7.13)$$

This equation asserts that for independent variations about the exact solutions the stationary character of $\lambda\{v_1, \varepsilon\}$ implies the same for the functional $I\{v_1, v\}$ and conversely.

It must be borne in mind that ε and v are related by equation (2.7.2). Because of this the same trial function used in both variational principles

will in general give different approximations. This was found to be the case for a Born trial field.

The relationship between these variational principles which was established above needs but little alteration to be made quite general. The proof above depended on the knowledge of the explicit form for $G(k_1 k_2; k_1' k_2')$. But this is unnecessary although it serves the purpose of giving motivation to the proof. Start with equations (2.7.1) and (2.7.2). Equation (2.7.11) follows as before with no restrictions on V nor the need for an explicit expression for G . The remainder of the argument is the same and leads to (2.7.13). The interpretation of this result is as before.

Appendix III contains the general proof outlined above. Both Kohn (see footnote 12) and Kato (see footnote 14) have obtained this relationship for two body problems.

Before proceeding to a discussion of a problem involving identical particles it is desirable to summarize the results obtained thus far.

An exact solution to a three body problem consisting of distinguishable interacting particles has been found. The Born expansion for this problem, which consists of the Born approximation and all higher order terms, can be evaluated and it converges to the exact solution. However, the Born approximation does not have a useful domain of applicability for any value of the total energy unless the interaction between the particles is very weak and the total energy is large. But when the second order term in the Born expansion is included, a useful domain of applicability is found to exist for large values of the energy and there is then no restriction on the magnitude of the interaction between the particles. This result implies that in general more terms in the Born expansion must

be evaluated beyond the Born approximation if useful results are to be obtained. In practice this is difficult to do. Two variational procedures are then considered. The Hulthén-Kohn variational principle limited in application to Born trial functions leads to the same results as the Born approximation. The Schwinger variational principle similarly restricted can give excellent or very poor results depending on the particular Born trial function used. The problem here is to supply some guide in choosing a good trial function. In practice the use of other than Born type trial functions in the Schwinger variational principle leads to very complicated mathematical computations which severely restrict the application of this procedure. On the other hand, the Hulthén-Kohn variational principle is more amenable to mathematical calculation than the Schwinger variational principle. Limited to Born type trial functions, the potentialities of the Hulthén-Kohn method were not fully exploited. However, the relationship between the Schwinger and Hulthén-Kohn variational principles which was known to exist for two body problems was indicated by the study to hold for three body problems and a general proof of this relationship for many body problems resulted.

Chapter III

IDENTICAL PARTICLES - SYMMETRIC PERTURBATION

3.1 Statement of the Problem

The system which was studied in Chapter II is now altered by permitting particle 1 to interact with the center of force and changing the energy of interaction between the incident and bound particles. These changes result in replacing the former distinguishable particles with identical ones.

The Schrodinger equation which describes this system is (3.1.1)

$$\left\{ \frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} - 2B\delta(x_1) - 2B\delta(x_2) + V(x_1 x_2) \right\} \psi(x_1 x_2) = E\psi(x_1 x_2).$$

All the quantities appearing in (3.1.1) have the same significance ascribed to them as in section (2.1). The momentum representation is obtained in a manner completely analogous to the procedure of section (2.1). Retaining the notation of that section, we find that (3.1.1) becomes

(3.1.2)

$$(k_1^2 + k_2^2 - E)f(k_1 k_2) - (B/\pi) \int f(k_1 k_2) dk_2 - (B/\pi) \int f(k_1 k_2) dk_1 \\ + (1/4\pi^2) \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f(k_1' k_2') = 0.$$

To complete the mathematical description of this system, the interaction kernel is assumed to be

(3.1.3)

$$(k_1 k_2 | V | k_1' k_2') = 2ATi \left\{ \frac{k_1 - k_1'}{(k_1^2 + T^2)(k_1'^2 + T^2)} + \frac{k_2 - k_2'}{(k_2^2 + T^2)(k_2'^2 + T^2)} \right\},$$

where A, the interaction strength, and T are real arbitrary constants.

The interaction, as (3.1.3) will be designated in what follows, is symmetric

in the interchange of particles 1 and 2 and is also hermitian, i.e.,

$$(k_1 k_2 | V | k'_1 k'_2) = (k'_2 k'_1 | V | k_2 k_1) \quad (3.1.4)$$

and

$$(k_1 k_2 | V | k'_1 k'_2) = (k'_1 k'_2 | V | k_1 k_2)^*. \quad (3.1.5)$$

In coordinate space this interaction is represented by an integral operator which has as its kernel the expression

$$\begin{aligned} A \left[\delta(x_2) \mathcal{V}(-x_1) \exp(Tx_1) \delta(x'_2) \mathcal{V}(-x'_1) \exp(Tx'_1) \right. \\ \left. - \delta(x_2) \mathcal{V}(x_1) \exp(-Tx_1) \delta(x'_2) \mathcal{V}(x'_1) \exp(-Tx'_1) \right. \\ \left. + \delta(x_1) \mathcal{V}(-x_2) \exp(Tx_2) \delta(x'_1) \mathcal{V}(-x'_2) \exp(Tx'_2) \right. \\ \left. - \delta(x_1) \mathcal{V}(x_2) \exp(-Tx_2) \delta(x'_1) \mathcal{V}(x'_2) \exp(-Tx'_2) \right], \end{aligned}$$

in which

$$\mathcal{V}(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}$$

This interaction is similar to that used for the preceding problem involving distinguishable particles. The form chosen here is based upon the same considerations as those given for the choice of the interaction (2.1.5) of section (2.1). This latter interaction cannot be used here because as we have seen the Schwinger variational principle is then independent of symmetric or antisymmetric trial functions and for identical particles the solutions of physical interest are just those with this kind of symmetry. It is for this reason that the interaction must be altered.

The physical problem which is mathematically represented by equations (3.1.2) and (3.1.3) differs from that considered in Chapter II by the occurrence of exchange phenomena. In other respects the two problems are similar. The exact solution of (3.1.2) is desired when the initial state of the system describes an incident particle from the left with momentum K_0 and a particle bound to the center of force. Although the physically interesting solutions are the symmetric and antisymmetric ones, so that the Pauli exclusion principle is satisfied, it is better for our purposes

to obtain the solution for the initial state described above. Then this solution can be symmetrized. Once the exact solution has been determined, the various scattering cross sections are to be calculated.

The approximation methods are also to be applied to this problem. This can be done in two distinct ways. The first of these will be considered in this chapter and consists in taking the last term on the left hand side of equation (3.1.2) as the perturbation. For an obvious reason, this procedure will be referred to as the symmetric perturbation. The second method which will be considered in detail in the following chapter regards the last two terms on the left hand side of (3.1.2) as the perturbation and in this form it will be referred to as the asymmetric perturbation. It is this method which is generally found in the literature (see footnote 1).

The approximation methods will be used to determine the various cross sections and these will then be compared with the exact values.

3.2 The Exact Solution

The direct method of solution does not readily yield the answer to this problem. However, the expansion method and the Green's function technique can both be used. The expansion method will be used to determine the Green's function and then the latter will be used to obtain the exact solution. In this way the details of both methods are simultaneously exhibited and previous results can be used.

The Green's function $G(k_1 k_2; k'_1 k'_2)$ is that solution of

$$\begin{aligned} (k_1^2 + k_2^2 - E)G(k_1 k_2; k'_1 k'_2) - (B/\pi) \int G(k_1 k_2; k'_1 k'_2) dk_1 - (B/\pi) \int G(k_1 k_2; k'_1 k'_2) dk_2 = \\ = \delta(k_1 - k'_1) \delta(k_2 - k'_2) \end{aligned} \quad (3.2.1)$$

which represents outgoing waves in coordinate space. The eigenfunctions in terms of which the solution of (3.2.1) is to be expanded are the solutions of the unperturbed equation

$$(k_1^2 + k_2^2 - E)f(k_1, k_2) - (B/\pi) \int f(k_1, k_2) dk_1 - (B/\pi) \int f(k_1, k_2) dk_2 = 0, \quad (3.2.2)$$

which represent an incident and outgoing wave in coordinate space.

Equation (3.2.2) is separable. Let

$$f(k_1, k_2) = f_1(k_1)f_2(k_2) \quad (3.2.3)$$

then f_1 and f_2 satisfy the equations,

$$(k_1^2 - K_1^2)f_1(k_1) - (B/\pi)C = 0, \quad (3.2.4)$$

$$(k_2^2 - K_2^2)f_2(k_2) - (B/\pi)D = 0$$

where

$$C = \int f_1(k_1) dk_1 \quad \text{and} \quad D = \int f_2(k_2) dk_2 \quad (3.2.5)$$

and $K_1^2 + K_2^2 = E$. K_1^2 is the energy of particle 1 and K_2^2 is the energy of particle 2. The eigenfunctions of the second of equations (3.2.4) have already been determined. These were given in equations (2.2.6), (2.2.7), and (2.2.23). The eigenfunctions of the first of these equations follows by replacing k_2 and K_2 with k_1 and K_1 respectively in the eigenfunctions for the second equation.

Hence the eigenfunctions for equation (3.2.2) are:

(3.2.6)

$$(K_1 K_2 | k_1 k_2) \equiv \left\{ \delta(k_1 - K_1) + \frac{B}{\pi} \frac{|K_1|}{|K_1| - Bi} \frac{1}{k_1^2 - K_1^2 - i\alpha} \right\} \\ \cdot \left\{ \delta(k_2 - K_2) + \frac{B}{\pi} \frac{|K_2|}{|K_2| - Bi} \frac{1}{k_2^2 - K_2^2 - i\alpha} \right\}; \quad (K_1^2 + K_2^2 = E),$$

$$(K_1 2 | k_1 k_2) \equiv \left\{ \delta(k_1 - K_1) + \frac{B}{\pi} \frac{|K_1|}{|K_1| - Bi} \frac{1}{k_1^2 - K_1^2 - i\alpha} \right\} \frac{N}{k_2^2 + B^2}; \quad K_1^2 = B^2 + E,$$

$$(1 K_2 | k_1 k_2) \equiv \left\{ \delta(k_2 - K_2) + \frac{B}{\pi} \frac{|K_2|}{|K_2| - Bi} \frac{1}{k_2^2 - K_2^2 - i\alpha} \right\} \frac{N}{k_1^2 + B^2}; \quad K_2^2 = B^2 + E,$$

$$(12 | k_1 k_2) \equiv N^2 / (k_1^2 + B^2)(k_2^2 + B^2), \quad E = -2B^2.$$

The following identities follow from (3.2.6)

$$(K_1 K_2 | k_1 k_2) = (K_2 K_1 | k_2 k_1), \quad (3.2.7)$$

$$(K_1 2 | k_1 k_2) = (1 K_1 | k_2 k_1),$$

$$(12 | k_1 k_2) = (12 | k_2 k_1).$$

The orthogonality relations satisfied by the eigenfunctions (3.2.6) are

$$\int (K_1' K_2' | k_1 k_2)^* dk_1 dk_2 (K_1 K_2 | k_1 k_2) = \delta(K_1 - K_1') \delta(K_2 - K_2'), \quad (3.2.8)$$

$$\int (K_1' 2 | k_1 k_2)^* dk_1 dk_2 (K_1 2 | k_1 k_2) = \delta(K_1 - K_1'),$$

$$\int (1 K_2' | k_1 k_2)^* dk_1 dk_2 (1 K_2 | k_1 k_2) = \delta(K_2 - K_2'),$$

$$\int (12 | k_1 k_2)^* dk_1 dk_2 (12 | k_1 k_2) = 1$$

All other products vanish. The closure property is also satisfied, i.e.,

(3.2.9)

$$\int (K_1 K_2 | k_1' k_2')^* dK_1 dK_2 (K_1 K_2 | k_1 k_2) + \int (K_1 2 | k_1' k_2')^* dK_1 (K_1 2 | k_1 k_2) + \\ \int (1 K_2 | k_1' k_2') dK_2 (1 K_2 | k_1 k_2) + (1 2 | k_1' k_2')^* (1 2 | k_1 k_2) = \delta(k_1 - k_1') \delta(k_2 - k_2').$$

Therefore the eigenfunctions (3.2.6) form a complete set.

Now expand the Green's function in terms of these eigenfunctions.

(3.2.10)

$$G(k_1 k_2; k_1' k_2') = \int G(K_1 K_2) dK_1 dK_2 (K_1 K_2 | k_1 k_2) + \int G(K_1) dK_1 (K_1 2 | k_1 k_2) \\ + \int G(K_2) dK_2 (1 K_2 | k_1 k_2) + G(1 2) (1 2 | k_1 k_2).$$

The functions $G(K_1 K_2)$, $G(K_1)$, $G(K_2)$ and $G(1 2)$ are the expansion coefficients and are distinct functions which have been distinguished for purposes of brevity from each other by their arguments.

The procedure for the determination of these coefficients is exactly the same as that given in section (2.2.2). The result of the calculation yields

(3.2.11)

$$G(K_1 K_2) = (K_1 K_2 | k_1' k_2')^* / (K_1^2 + K_2^2 - E), \\ G(K_1) = (K_1 2 | k_1' k_2')^* / (K_1^2 - K_0^2); K_0^2 = B^2 + E \\ G(K_2) = (1 K_2 | k_1' k_2')^* / (K_2^2 - K_0^2); \\ G(1 2) = -(1 2 | k_1' k_2')^* / (E_0^2 + B^2).$$

From (3.2.10) and (3.2.11) the Green's function becomes

(3.2.12)

$$G(k_1 k_2; k_1' k_2') = \int \frac{(K_1 K_2 | k_1' k_2')^* dK_1 dK_2 (K_1 K_2 | k_1 k_2)}{K_1^2 + K_2^2 - E}$$

$$\begin{aligned}
 & + \int \frac{(K_1 2 | k_1' k_2')^* dK_1 (K_1 2 | k_1 k_2)}{K_1^2 - K_0^2} \\
 & + \int \frac{(1K_2 | k_1' k_2')^* dK_2 (1K_2 | k_1 k_2)}{K_2^2 - K_0^2} \\
 & - \frac{(12 | k_1' k_2')^* (12 | k_1 k_2)}{K_0^2 + B^2} .
 \end{aligned}$$

The identities (3.2.7) coupled with equation (3.2.12) yield

$$G(k_1 k_2; k_1' k_2') = G(k_2 k_1; k_2' k_1'). \quad (3.2.13)$$

From the orthogonality and closure relations we see that the complex conjugates of the eigenfunctions also form a complete set. Thus the Green's function of equation (3.2.2) could be obtained as an expansion in terms of the complex conjugates of the eigenfunctions. Therefore it follows from (3.2.12) that

$$G(k_1 k_2; k_1' k_2') = G(k_1' k_2'; k_1 k_2). \quad (3.2.14)$$

In terms of the Green's function, the solution of equation (3.1.2) may be represented by the integral equation

$$f(k_1 k_2) = f_0(k_1 k_2) - (1/4\pi^2) \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2''), \quad (3.2.15)$$

where $f_0(k_1 k_2)$ is the solution of the unperturbed wave equation which describes the initial state of the system. Substitute the interaction (3.1.3) into (3.2.15) and evaluate. The result is

$$f(k_1 k_2) = f_0(k_1 k_2) - (2ATi/4\pi^2) \left[I_1 C_1 + I_2 C_2 - I_3 D_1 - I_4 D_2 \right], \quad (3.2.16)$$

where

(3.2.17)

$$I_1 = I_1(k_1 k_2) = \int G(k_1 k_2; k_1' k_2') k_1' dk_1' dk_2' / (k_1'^2 + T^2),$$

$$I_2 = I_2(k_1 k_2) = \int G(k_1 k_2; k_1' k_2') k_2' dk_1' dk_2' / (k_2'^2 + T^2),$$

$$I_3 = I_3(k_1 k_2) = \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' / (k_1'^2 + T^2),$$

$$I_4 = I_4(k_1 k_2) = \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' / (k_2'^2 + T^2),$$

and

$$C_1 = \int f(k_1 k_2) dk_1 dk_2 / (k_1^2 + T^2); \quad C_2 = \int f(k_1 k_2) dk_1 dk_2 / (k_2^2 + T^2) \quad (3.2.18)$$

$$D_1 = \int f(k_1 k_2) k_1 dk_1 dk_2 / (k_1^2 + T^2); \quad D_2 = \int f(k_1 k_2) k_2 dk_1 dk_2 / (k_2^2 + T^2).$$

The constants C_1 , C_2 , D_1 , and D_2 can be determined from equations (3.2.16) and (3.2.18).

To simplify the calculations the following integral operators are defined. For arbitrary functions $f(k_1 k_2)$ let,

$$P_1(f) \equiv \int f(k_1 k_2) dk_1 dk_2 / (k_1^2 + T^2), \quad (3.2.19)$$

$$P_2(f) \equiv \int f(k_1 k_2) dk_1 dk_2 / (k_2^2 + T^2)$$

$$P_3(f) \equiv \int f(k_1 k_2) k_1 dk_1 dk_2 / (k_1^2 + T^2),$$

and

$$P_4(f) \equiv \int f(k_1 k_2) k_2 dk_1 dk_2 / (k_2^2 + T^2).$$

Then from (3.2.18) and (3.2.16) we obtain

$$C_1 = P_1(f_0) + \ell [P_1(I_3)D_1 + P_1(I_4)D_2] , \quad (3.2.20)$$

$$C_2 = P_2(f_0) + \ell [P_1(I_4)D_1 + P_1(I_3)D_2] ,$$

$$D_1 = P_3(f_0) - \ell [P_3(I_1)C_1 + P_3(I_2)C_2] ,$$

and

$$D_2 = P_4(f_0) - \ell [P_3(I_2)C_1 + P_3(I_1)C_2] ,$$

in which $\ell \equiv 2\Delta\tau/4\pi^2$. This simplification results when the symmetry properties of the Green's function, equations (3.2.13) and (3.2.14), are used and the fact that $P_1(I_1) = P_1(I_2) = P_3(I_3) = P_3(I_4) = 0$.

The values of the constants are

$$C_1 = C_{11} + C_{12} , \quad C_2 = C_{11} - C_{12} \quad (3.2.21)$$

where

$$2C_{11} = \left\{ P_1(f_0) + P_2(f_0) + \ell P_1(I_3+I_4) [P_3(f_0) + P_4(f_0)] \right\} \Delta_1 , \quad (3.2.22)$$

$$\Delta_1^{-1} = 1 + \ell^2 P_1(I_3 + I_4) P_3(I_1 + I_2) ,$$

$$2C_{12} = \left\{ P_1(f_0) - P_2(f_0) + \ell P_1(I_3-I_4) [P_3(f_0) - P_4(f_0)] \right\} \Delta_2 , \quad (3.2.23)$$

$$\Delta_2 = 1 + \ell^2 P_1(I_3 - I_4) P_3(I_1 - I_2) ,$$

and

$$D_1 = D_{11} + D_{12} , \quad D_2 = D_{11} - D_{12} , \quad (3.2.24)$$

where

$$2D_{11} = \left\{ P_3(f_0) + P_4(f_0) - \ell P_3(I_1+I_2) [P_1(f_0) + P_2(f_0)] \right\} \Delta_1 \quad (3.2.25)$$

$$2D_{12} = \left\{ P_3(f_0) - P_4(f_0) - \ell P_3(I_1-I_2) [P_1(f_0) - P_2(f_0)] \right\} \Delta_2 . \quad (3.2.26)$$

Hence equation (3.2.16) may be written

$$f(k_1 k_2) = f_0(k_1 k_2) - \ell [C_{11}(I_1+I_2) + C_{12}(I_1-I_2) - D_{11}(I_3+I_4) - D_{12}(I_3-I_4)] . \quad (3.2.27)$$

From (3.2.17) and (3.2.13) it follows that

$$I_2(k_1 k_2) = I_1(k_2 k_1) \quad \text{and} \quad I_4(k_1 k_2) = I_3(k_2 k_1) \quad (3.2.28)$$

Since $f_0(k_1 k_2)$ may be written

$$f_0(k_1 k_2) = \frac{1}{2} [f_0(k_1 k_2) + f_0(k_2 k_1)] + \frac{1}{2} [f_0(k_1 k_2) - f_0(k_2 k_1)] , \quad (3.2.29)$$

equation (3.2.27) represents the solution $f(k_1 k_2)$ as a sum of a symmetric and antisymmetric function. The symmetric function is

$$f_s(k_1 k_2) = \frac{1}{2} [f_0(k_1 k_2) + f_0(k_2 k_1)] - \ell [C_{11}(I_1 + I_2) - D_{11}(I_3 + I_4)] , \quad (3.2.30)$$

and the antisymmetric function is

$$f_a(k_1 k_2) = \frac{1}{2} [f_0(k_1 k_2) - f_0(k_2 k_1)] - \ell [C_{12}(I_1 - I_2) - D_{12}(I_3 - I_4)] , \quad (3.2.31)$$

The initial state $f_0(k_1 k_2)$ has not been specified. If $f_0(k_1 k_2)$ is symmetric then $C_{12} = D_{12} = 0$ because $P_1(f_0) = P_2(f_0)$ and $P_3(f_0) = P_4(f_0)$. Then for a symmetric initial state the solution is just $f_s(k_1 k_2)$ given by (3.2.30). Similarly if the initial state $f_0(k_1 k_2)$ is antisymmetric the solution $f(k_1 k_2)$ reduces to $f_a(k_1 k_2)$.

The solutions of physical interest are the symmetric and antisymmetric ones. In particular, our interest centers around the scattered waves associated with these solutions. The scattered waves are the asymptotic parts of the solutions and these are the following expressions:

$$(3.2.32)$$

$$f(k_1 k_2) \sim (2)^{-1/2} \left[\delta(k_1 - K_0) \frac{N}{k_2^2 + B^2} \pm \delta(k_2 - K_0) \frac{N}{k_1^2 + B^2} \right]$$

$$\begin{aligned}
 & + \left[\frac{B}{\pi(2)^{1/2}} \frac{K_o}{K_o - B_1} - \frac{N\pi}{B} \ell \left\{ \frac{Ck_1}{K_o^2 + T^2} - \frac{D}{T(T+B)} \frac{K_o}{K_o - B_1} \left(\frac{T^2 - B^2}{K_o^2 + T^2} \pm 1 \right) \right\} \right] \frac{N}{(k_2^2 + B^2)(k_1^2 - K_o^2)} \\
 & \pm \left[\frac{B}{\pi(2)^{1/2}} \frac{K_o}{K_o - B_1} - \frac{N\pi}{B} \ell \left\{ \frac{Ck_2}{K_o^2 + T^2} - \frac{D}{T(T+B)} \frac{K_o}{K_o - B_1} \left(\frac{T^2 - B^2}{K_o^2 + T^2} \pm 1 \right) \right\} \right] \frac{N}{(k_1^2 + B^2)(k_2^2 - K_o^2)} \\
 & - \ell \left[C \left(\frac{k_1 |k_2|}{(k_1^2 + T^2)(|k_2| - B_1)} \pm \frac{k_2 |k_1|}{(k_2^2 + T^2)(|k_1| - B_1)} \right) \right. \\
 & \quad \left. - D \frac{(T-B)}{T} \frac{|k_1| |k_2|}{(|k_1| - B_1)(|k_2| - B_1)} \left(\frac{1}{k_1^2 + T^2} \pm \frac{1}{k_2^2 + T^2} \right) \right] \frac{1}{k_1^2 + k_2^2 - E}.
 \end{aligned}$$

In this equation, the plus sign in \pm refers to the symmetric solution and the minus sign to the antisymmetric solution. C and D represent the values for the constants C_{11} , C_{12} , D_{11} , and D_{12} which must be associated with these solutions and which are given by equations (3.2.30) and (3.2.31). The initial state for which (3.2.32) is the solution is

$$\begin{aligned}
 f_o(k_1 k_2) = (2)^{-1/2} & \left[\left\{ \delta(k_1 - K_o) + \frac{B}{\pi} \frac{K_o}{K_o - B_1} \frac{1}{k_1^2 - K_o^2} \right\} \frac{N}{k_2^2 + B^2} \right. \\
 & \left. \pm \left\{ \delta(k_2 - K_o) + \frac{B}{\pi} \frac{K_o}{K_o - B_1} \frac{1}{k_2^2 - K_o^2} \right\} \frac{N}{k_1^2 + B^2} \right]
 \end{aligned} \tag{3.2.33}$$

The first term on the right hand side of (3.2.32) represents that portion of the incident wave which is unaltered by the interaction with the "atom." The second term represents the elastic scattering of particles 1 which is composed of the direct scattering of the incident particles 1 plus the exchange scattering of the incident particles 2 with the bound particles 1. The third term represents the elastic scattering of particles 2 and describes the same physical phenomena just given for

particles 1. The fourth term on the right hand side of (3.2.32) represents the inelastic scattering of the incident particles 1 and 2.

Following the same procedure given in Chapter II for distinguishable particles we calculate the various cross sections—elastic and inelastic. The elastic scattering cross section for particles 1 or 2 is given by

$$Q_e = (\pi^2/K_0^2) \left[|C(K_0)|^2 + |C(-K_0)|^2 \right] \quad (3.2.34)$$

$$(3.2.35)$$

where

$$C(\pm K_0) \equiv \frac{B}{\pi(2)^{1/2}} \frac{K_0}{K_0 - Bi} - \frac{N\pi}{B} \ell \left\{ \pm \frac{CK_0}{K_0^2 + T^2} - \frac{D}{T(B+T)} \frac{K_0}{K_0 - Bi} \left(1 + \frac{T^2 - B^2}{K_0^2 + T^2} \right) \right\},$$

for the symmetric wave function. $C(\pm K_0)$ for the antisymmetric solution is given by the same expression except that +1, the last term in parenthesis in the curly brackets, must be replaced by -1. The constants C and D must be those that are to be associated with the symmetric or antisymmetric solutions. The inelastic scattering cross section is

$$Q_i = -(2\pi^2 \ell^2/K_0) \left[|C|^2 J_1 + |D|^2 (T-B)^2 (J_2/T^2) \right], \quad E > 0 \quad (3.2.36)$$

Here

$$J_1 = \frac{\pi}{K_0^2 + T^2} \frac{TK_0^2}{(T^2 + E)^{1/2}} \left(\frac{B}{K_0} - \frac{(T^2 + E)^{1/2}}{T} \right)^2, \quad E > 0 \quad (3.2.37)$$

which is the same for both the symmetric and antisymmetric solutions and

$$J_2 = \int_{-\sqrt{E}}^{+\sqrt{E}} \frac{(E - k_2^2)^{1/2} k_2^2 dk_2}{(K_0^2 - k_2^2)(k_2^2 + B^2)} \left(\frac{1}{k_1^2 + T^2} \pm \frac{1}{k_2^2 + T^2} \right)^2, \quad E > 0 \quad (3.2.38)$$

The \pm sign has the same meaning as before.

Equations (3.2.37) and (3.2.38) show that if $E = 0$, then $Q_1 = 0$ whatever the values C and D may have. This of course is physically necessary and is similar to the situation which arose in the discussion of the problem for distinguishable particles.

The continuity equation leads to the relation

$$Q_0 + Q_1/2 = K_0^{-1} \operatorname{Im} \left\{ \pi(2)^{1/2} c(K_0) \right\}. \quad (3.2.39)$$

This equation is used to check the numerical calculations. Its significance has been fully discussed in section (2.3).

3.3 The Born Approximation

In analogy to the development given in section (2.4), it is expedient to consider the solution of (3.1.2) as a power series--the Born expansion--in the interaction strength A .

Let

$$f(k_1 k_2) = \sum_{n=0}^{\infty} A^n f_n(k_1 k_2). \quad (3.3.1)$$

Substitute (3.3.1) into (3.1.2) and equate the coefficients of like powers of A . We obtain the following set of equations:

For $n=0$

$$(k_1^2 + k_2^2 - E) f_0(k_1 k_2) - (B/\pi) \int f_0(k_1 k_2) dk_1 - (B/\pi) \int f_0(k_1 k_2) dk_2 = 0, \quad (3.3.2)$$

and for $n \geq 1$

$$\begin{aligned} (k_1^2 + k_2^2 - E) f_n(k_1 k_2) - (B/\pi) \int f_n(k_1 k_2) dk_1 - (B/\pi) \int f_n(k_1 k_2) dk_2 \\ = - (1/4\pi^2) \int V |dk_1' dk_2'| f_{n-1}(k_1' k_2') \end{aligned} \quad (3.3.3)$$

where

$$AV' \equiv (k_1 k_2 | V | k_1' k_2').$$

Equation (3.3.2) represents the unperturbed system as a comparison with (3.2.2) reveals. The physical situation described by this equation is that in which particles 1 and 2 interact with the center of force but not with each other. Thus the solution of this equation represents the initial state of the system. Equations (3.3.3) represent the contributions to the wave function that arise from the interaction between the particles. Physically the solutions of these equations must represent outgoing particles in coordinate space.

The Born approximation consists in the evaluation of the terms $n = 0, 1$. This will be considered below.

Equations (3.3.3) are solved by the Green's function technique. The result for $n \geq 1$ is

$$f_n(k_1 k_2) = -m \left[I_1 P_1(f_{n-1}) + I_2 P_2(f_{n-2}) - I_3 P_3(f_{n-1}) - I_4 P_4(f_{n-1}) \right], \quad (3.3.4)$$

where $m = 2T_1/4\pi^2$ and the notation of the preceding section has been used. From this equation and the relations $P_1(I_1) = P_1(I_2) = P_3(I_3) = P_3(I_4) = 0$, we find that

$$P_1(f_n) = m \left[P_1(I_3) P_3(f_{n-1}) + P_1(I_4) P_4(f_{n-1}) \right], \quad (3.3.5)$$

$$P_2(f_n) = m \left[P_1(I_4) P_3(f_{n-1}) + P_1(I_3) P_4(f_{n-1}) \right],$$

$$P_3(f_n) = -m \left[P_3(I_1) P_1(f_{n-1}) + P_3(I_2) P_2(f_{n-1}) \right],$$

and

$$P_4(f_n) = -m \left[P_3(I_2) P_1(f_{n-1}) + P_3(I_1) P_2(f_{n-1}) \right].$$

These equations (3.3.4) and (3.3.5) may be written in matrix notation and become

$$f_n(k_1 k_2) = -m I R_{n-1} = -m I \alpha^{n-1} R_0, \quad (3.3.6)$$

$$R_n = \alpha R_{n-1} = \alpha^n R_0, \quad (3.3.7)$$

in which

$$I = (I_1, I_2, -I_3, -I_4),$$

$$R_n = \begin{pmatrix} P_1(f_n) \\ P_2(f_n) \\ P_3(f_n) \\ P_4(f_n) \end{pmatrix}$$

and

$$\alpha = m \begin{pmatrix} 0 & 0 & P_1(I_3) & P_1(I_4) \\ 0 & 0 & P_1(I_4) & P_1(I_3) \\ -P_3(I_1) & -P_3(I_2) & 0 & 0 \\ -P_3(I_2) & -P_3(I_1) & 0 & 0 \end{pmatrix}$$

Substitute (3.3.6) into (3.3.1). Then

$$f(k_1 k_2) = f_0(k_1 k_2) - \ell I(1 - A\alpha)^{-1} R_0. \quad (3.3.8)$$

The evaluation of this equation gives the exact solution—equation (3.2.16).

Therefore the Born expansion converges to the exact solution. However, the series representation of the exact solution is valid only within its radius of convergence. The latter is determined by those values of the elements of the matrix $(1-A\alpha)$ such that its inverse exists. In other words the smallest in absolute value of the roots of $\det.(1-A\alpha) = 0$ will yield the radius of convergence.

Explicitly the radius of convergence of the Born expansion (3.3.1) is given by the smallest in absolute value of the roots for A of

$$\Delta \equiv \left[1 + \ell^2 P_1(I_3 - I_4) P_3(I_1 - I_2) \right] \left[1 + \ell^2 P_1(I_3 + I_4) P_3(I_1 + I_2) \right] = 0, \quad (3.3.9)$$

where $\ell = 2iAT/4\pi^2$. In the notation of the preceding section

$$\Delta = (\Delta_1 \Delta_2)^{-1}. \text{ No restrictions have been placed on the initial state}$$

$f_0(k_1 k_2)$ in the derivation of (3.3.8). The result is then applicable if $f_0(k_1 k_2)$ is chosen symmetric or antisymmetric. The series representing either of these solutions have different radii of convergence. Thus for the symmetric solution $P_1(I_3 - I_4) = P_3(I_1 - I_2) = 0$ and the radius of convergence is determined by

$$\Delta_1^{-1} = 1 + \ell^2 P_1(I_3 + I_4) P_3(I_1 + I_2) = 0.$$

For the antisymmetric solution it is determined by $\Delta_2^{-1} = 0$. It is apparent that in general the radius of convergence of a series representation of a general solution of (3.3.1) is the smaller of the radii of convergence of the symmetric and antisymmetric solutions. It follows that if such a solution is symmetrized the resulting function is limited by the smaller of the two radii of convergence. On physical grounds one would expect the antisymmetric solution to have a larger radius of convergence than the symmetric solution because for the former the wave function is small when the interaction between the particles is large. The net result is to have an effective interaction which is weaker than the actual interaction. If we form an antisymmetric solution from a general solution (in series representation), the resulting function may be valid over a larger range of values than the general solution. In general, when spin is taken into account both symmetric and antisymmetric functions are needed. If reliable experimental data is on hand, then a better estimation of the effect of the symmetric wave function can be obtained by calculating the contribution from the antisymmetric wave function and subtracting its value from the experimental data.

The Born approximation is given by

$$\begin{aligned} f_B(k_1 k_2) &= f_o(k_1 k_2) + A f_1(k_1 k_2) \\ &= f_o(k_1 k_2) - \ell \left[I_1 P_1(f_o) + I_2 P_2(f_o) - I_3 P_3(f_o) - I_4 P_4(f_o) \right]. \end{aligned} \quad (3.3.10)$$

For a symmetric or antisymmetric initial state $f_o(k_1 k_2)$, i.e., equation (3.2.33), the above equation gives the following approximations to the exact constants C_{11} , D_{11} , C_{12} , and D_{12} : For the symmetric solution

$$C_{11B} = P_1(f_{os}) = (2)^{-1/2} \frac{N\pi}{BT} \frac{K_o}{K_o - Bi} \left[\frac{T-B}{K_o^2 + T^2} + \frac{1}{T+B} \right], \quad (3.3.11)$$

$$D_{11B} = P_3(f_{os}) = (2)^{-1/2} \frac{N\pi}{B} \frac{K_o}{K_o^2 + T^2};$$

For the antisymmetric solution,

$$C_{12B} = P_1(f_{oa}) = (2)^{-1/2} \frac{N\pi}{BT} \frac{K_o}{K_o - Bi} \left[\frac{T-B}{K_o^2 + T^2} - \frac{1}{T+B} \right], \quad (3.3.12)$$

$$D_{12B} = P_3(f_{oa}) = (2)^{-1/2} \frac{N\pi}{B} \frac{K_o}{K_o^2 + T^2}.$$

Here f_{os} and f_{oa} are the symmetric and antisymmetric initial states of the system. These values for the constants C and D are equal to the exact values provided that A is very small or that the products $AP_1(I_3 \pm I_4)$ and $AP_3(I_1 \pm I_2)$ are very small. This situation is similar to that found for the problem of distinguishable particles. It implies that the Born approximation is valid if the interaction is weak and the total energy is large.

The dependence of the radius of convergence on the total energy, E, of the system is

$$\rho = T(E)^{1/2} / \pi \quad (3.3.13)$$

for large values of E. For convenience we have taken ρ expressed in

terms of $|A/4\pi|$. This relation holds for both the symmetrical and anti-symmetrical solutions. It is also identical with (2.4.23) which was obtained for distinguishable particles. Therefore the conclusions drawn there are valid here also.

The general features of this iteration procedure are the same as those discussed in section (2.4) and the results of that discussion can be carried over.

The Born approximation for arbitrary values of A can readily be considered. For large values of the total energy E, the values for the exact constants C and D are

$$C = \pm (2)^{-1/2} \quad N\pi/BT(T+B) \quad (3.3.14)$$

$$D = (2)^{-1/2} \quad \frac{N\pi}{B} \quad \frac{K_o}{K_o^2 + T^2} \left(1 \pm \frac{A}{4\pi} \cdot \frac{\pi}{T(T+B)} - \right).$$

Under the same conditions, the scattering cross sections become

$$Q_i = (8\pi T/E)(A/4\pi)^2 |C|^2,$$

and

$$Q_e = B^2/E.$$

The Born approximation yields

$$C_B = C, \quad (3.3.15)$$

$$D_B = (2)^{-1/2} \quad \frac{N\pi}{B} \quad \frac{K_o}{K_o^2 + T^2}.$$

Since the constant D plays no role in determining the scattering cross section, we see that the Born result will be a good approximation to the exact result for this range of the energy. However, the scattering amplitudes depend on C and D and in this case we see that unless $A/4\pi \ll T(T+B)/\pi$ the Born result will not give good agreement with the exact scattering amplitudes even for large values of E.

The second Born approximation gives the following values for the constants C and D for large E,

$$C_{2B} = C ; \quad D_{2B} = D . \quad (3.3.16)$$

Here we see that both the scattering cross sections and scattering amplitudes obtained from the second Born approximation will give good agreement with the exact values for large values of E. This result is again similar to that obtained in the preceding chapter and the analysis there holds in the present case.

Table IV consists of the results of a numerical calculation of the scattering cross sections for the exact symmetric solution and for the associated Born approximation. The parameters have been chosen so that $A/4\pi = 1$ and $T = 2B$. For this value of the interaction strength A, the table indicates, as is to be expected from general considerations, that the Born approximation yields useful results only when the radius of convergence of the Born expansion for the symmetric solution, ρ_s , is greater than 1. For large values of the total energy E, the Born approximation approaches the exact values.

Table V contains the same information as Table IV, except that the calculations are for the antisymmetric solution. In this case the value assumed for A lies well within the radius of convergence ρ_a and the corresponding values for the quantities calculated are very good approximations to the exact result for all values of the energy.

These tables verify what has been said about the radii of convergence of the Born expansion for the symmetric and antisymmetric solutions. It is also clear that as the value for A increases larger values of E must be taken in order to obtain useful results from the Born approximation. The Born expansion, however, converges and here we meet again the same problem discussed in Chapter II. The analysis given there holds here also.

To utilize the Born expansion additional terms must be calculated and in practice this is very difficult to do. Variational procedures offer an approach which substantially reduces the mathematical calculations involved and we now turn to a study of such methods.

Table IV

SYMMETRIC PERTURBATION - SYMMETRIC SOLUTION

z	Exact		Born Approximation		
	Q_{eS}	Q_{iS}	ρ_S	Q_{eB}	Q_{iB}
-.9	.853805		1.06744	1.47820	
-.5	1.05210		.903667	2.27123	
-.1	1.10402		.925606	2.32585	
-.05	1.10477		.930891	2.31255	
-.01	1.10476		.935332	2.30006	
-.005	1.10473		.935894	2.29841	
-.001	1.10468		.936347	2.29703	
+.001	1.10467	$10^{-7}.147577$.936573	2.29633	$10^{-7}.175339$
+.005	1.10464	$10^{-6}.366396$.937026	2.29500	$10^{-6}.437171$
.01	1.10459	$10^{-4}.107206$.937594	2.29326	$10^{-5}.258133$
.05	1.10364	$10^{-3}.286340$.942112	2.27868	$10^{-3}.649928$
.1	1.10154	$10^{-2}.107717$.947773	2.25885	$10^{-2}.247901$
.5	1.06137	.017392	.990463	2.06239	.429422
.9	1.00185	.037187	1.03888	1.84770	.993868
5.	.518503	.106581	1.47143	.651187	.307757
10.	.284078	.107917	1.91763	.289203	.257411
100.	.015933	.036397	6.01935	.013138	.041558
1000.	.001053	.004302	20.0416	.001033	.004359

z = total energy E in units of the bound state energy B^2 .

Q_{eS} = elastic scattering cross section for symmetrical wave function.

Q_{eB} = elastic scattering cross section for Born approximation to symmetrical wave function.

Q_{iS} = inelastic scattering cross section for symmetrical wave function.

Q_{iB} = inelastic scattering cross section for Born approximation to symmetrical wave function.

$\rho_S = \left| \frac{A}{4\pi} \right|$ radius of convergence of Born expansion for symmetric wave function.

Table V

SYMMETRIC PERTURBATION - ANTISYMMETRIC SOLUTION

Exact Solution			Born Approximation		
z	Q _{ea}	Q _{ia}	ρ_a	Q _{eB}	Q _{iB}
-.9	.948379		1.75739	.922751	
-.5	.786795		1.78538	.730850	
-.1	.678528		1.82632	.630407	
-.05	.667623		1.83194	.621099	
-.01	.659256		1.83644	.614017	
-.005	.658233		1.83700	.613154	
-.001	.657397		1.83757	.612465	
+.001	.657011	10 ⁻⁷ .123372	1.83766	.612121	10 ⁻⁷ .109669
.005	.656205	10 ⁻⁶ .308733	1.83810	.611440	10 ⁻⁶ .274256
.01	.655196	10 ⁻⁵ .123441	1.83866	.610589	10 ⁻⁵ .109565
.05	.647282	10 ⁻⁴ .322985	1.84295	.603945	10 ⁻⁴ .297264
.1	.637722	10 ⁻³ .118526	1.84820	.596012	10 ⁻⁴ .995573
.5	.576029	10 ⁻² .298766	1.87063	.543805	10 ⁻² .248957
.9	.520376	10 ⁻² .879515	1.92261	.504394	10 ⁻² .730707
5.	.259111	.0877559	2.28234	.290243	.074559
10.	.147364	.118174	2.67852	.174831	.103738
100.	.012500	.038254	6.46166	.0127781	.0369564
1000.	.001016	.004322	20.2075	.00103251	.0043067

z = total energy E in units of the bound state energy B².

Q_{ea} = elastic scattering cross section for antisymmetric wave function.

Q_{eB} = elastic scattering cross section for Born approximation to antisymmetric wave function.

Q_{ia} = inelastic scattering cross section for antisymmetric wave function.

Q_{iB} = inelastic scattering cross section for Born approximation to antisymmetric wave function.

$\rho_a = \left| \frac{A}{4\pi} \right|$ = radius of convergence of Born expansion for antisymmetric wave function.

3.4 The Schwinger Variational Principle

Consider the integral equation representation of (3.1.2) which satisfies the initial conditions of the problem. This is

$$(3.4.1)$$

$$f(k_1 k_2) = f_0(k_1 k_2) - (1/4\pi^2) \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2'').$$

Here $f_0(k_1 k_2)$ describes the initial state of the system and is a solution of the unperturbed equation, i.e., equation (3.1.2) with the interaction set equal to zero.

In addition to (3.4.1), we consider the integral equation adjoint to it. This integral equation represents solutions of the wave equation in terms of incoming or concentrating waves. It is expressed in terms of the Green's function $G_0(k_1 k_2; k_1' k_2')$ which is related to that occurring in (3.4.1) as follows:

$$G_0(k_1 k_2; k_1' k_2') = G^*(k_1' k_2'; k_1 k_2) \quad (3.4.2)$$

This relation implies the same properties for G_0 which equations (3.2.13) and (3.2.14) express for G . The adjoint integral equation is

$$f_1(k_1 k_2) = f_{01}(k_1 k_2) - (1/4\pi^2) \int G_0(k_1 k_2; k_1' k_2') dk_1' dk_2' (k_1' k_2' | V | k_1'' k_2'') dk_1'' dk_2'' f_1(k_1'' k_2'') \quad (3.4.3)$$

which may be written

$$f_1(k_1 k_2) = f_{01}(k_1 k_2) - (1/4\pi^2) \int f_1(k_1'' k_2'') dk_1'' dk_2'' (k_1'' k_2'' | V | k_1' k_2')^* dk_1' dk_2' G^*(k_1' k_2'; k_1 k_2),$$

when (3.4.2) is used and the hermitian character of the interaction is taken into account. $f_{01}(k_1 k_2)$ are solutions of the unperturbed equation which will be specified below.

The integral equations (3.4.1) and (3.4.3) are treated in the same way as in Chapter II, section (2.6). The equations (2.6.3) to (2.6.13) inclusive may be taken over directly. The only changes that must be made in the application of these equations to this problem is the replacement

of the interaction and Green's function with the corresponding quantities associated with the present problem.

The Schwinger variational expression is

$$\lambda \{v_1, v\} = (v_1, Kv) / (v_1, P)(a_1, v). \quad (3.4.4)$$

Now

$$(a_1, f) = 2ATi \left[C_1 P_3(f_{01}^*) + C_2 P_4(f_{01}^*) - D_1 P_1(f_{01}^*) - D_2 P_2(f_{01}^*) \right], \quad (3.4.5)$$

is obtained from (2.6.14) by inserting the interaction and carrying through the integrations. The notation is that of section (3.2). This equation represents the exact value for (a_1, f) . The elements of (3.4.4) can also be evaluated and the results of the calculation are,

$$\begin{aligned} (v_1, Kv) = 2ATi & \left[P_3(v_1^*)P_1(v) - P_1(v_1^*)P_3(v) + P_4(v_1^*)P_2(v) - P_2(v_1^*)P_4(v) \right] \\ & - (ATi/\pi)^2 \left[P_3(v_1^*) \left\{ P_1(I_3)P_3(v) + P_1(I_4)P_4(v) \right\} \right. \\ & + P_1(v_1^*) \left\{ P_3(I_1)P_1(v) + P_3(I_2)P_2(v) \right\} \\ & + P_4(v_1^*) \left\{ P_1(I_4)P_3(v) + P_1(I_3)P_4(v) \right\} \\ & \left. + P_2(v_1^*) \left\{ P_3(I_2)P_1(v) + P_3(I_1)P_2(v) \right\} \right], \end{aligned} \quad (3.4.6)$$

$$(a_1, v) = 2ATi \left[P_1(v)P_3(f_{01}^*) + P_2(v)P_4(f_{01}^*) - P_3(v)P_1(f_{01}^*) - P_4(v)P_2(f_{01}^*) \right],$$

and

$$(v_1, a) = 2ATi \left[P_3(v_1^*)P_1(f_0) - P_1(v_1^*)P_3(f_0) + P_4(v_1^*)P_2(f_0) - P_2(v_1^*)P_4(f_0) \right]. \quad (3.4.8)$$

Equation (3.4.4) gives an approximation to (a_1, f) which in turn yields approximations to the exact constants C_1 , C_2 , D_1 , and D_2 .

The equations (3.4.6), (3.4.7) and (3.4.8) are general and no restrictions have been placed on the trial functions v and v_1 . The principle is to be used to obtain the scattering cross sections for the symmetric and antisymmetric solutions so that the trial functions v will be chosen to have the same symmetry properties as the solutions. There is no a priori reason for choosing v in this way. It might be argued that since the exact solutions have these symmetry properties then to obtain good approximations the trial functions should be "close" to the exact solutions. This implies that the trial functions should have the same symmetry properties as the exact solutions. However, in the problem for distinguishable particles, we found that "closeness" was an inadequate criterion and in fact found trial functions which could not be considered "close" to the exact solution but which nonetheless gave excellent results. Since Born trial functions of the symmetric or antisymmetric type are to be considered and since the exact solutions have these symmetries, we shall restrict v in this way but v_1 is to be arbitrary. With this restriction on v , we find that

(3.4.9)

$$\begin{aligned}
 (v_1, Kv) = & 2ATi \left[P_1(v) \left\{ P_3(v_1^*) \pm P_4(v_1^*) \right\} - P_3(v) \left\{ P_1(v_1^*) \pm P_3(v_1^*) \right\} \right] \\
 & - (ATi/\pi)^2 \left[P_3(v) \left\{ P_3(v_1^*) \pm P_4(v_1^*) \right\} P_1(I_3 \pm I_4) \right. \\
 & \left. + P_1(v) \left\{ P_1(v_1^*) \pm P_2(v_1^*) \right\} P_3(I_1 \pm I_2) \right] , \\
 (a_1, v) = & 2ATi \left[P_1(v) \left\{ P_3(f_{01}^*) \pm P_4(f_{01}^*) \right\} - P_3(v) \left\{ P_1(f_{01}^*) \pm P_2(f_{01}^*) \right\} \right] ,
 \end{aligned}$$

and

$$(v_1, a) = 2ATi \left[P_1(f_0) \left\{ P_3(v_1^*) \pm P_4(v_1^*) \right\} - P_3(f_0) \left\{ P_1(v_1^*) \pm P_2(v_1^*) \right\} \right] .$$

The plus sign in \pm is to be associated with the symmetric trial function v and the minus sign with the antisymmetric trial function. This convention will be adhered to in what follows. $f_0(k_1 k_2)$ is taken symmetric or antisymmetric since it represents the initial state of the system. Notice that the relations (3.4.9) in conjunction with (3.2.19) result in the symmetrization of v_i . Hence we may assume that v_i has the same symmetry properties as v .

If use is made of (2.6.13), equations (3.4.9) and (3.4.4) yield the exact values for the constants C_1 , C_2 , D_1 , and D_2 . For let $v = f$, then

$$\lambda \left\{ v_i, f \right\} = 1 / (a_i, f)$$

for arbitrary v_i . The left side of this equation can be found from (3.4.9) and the right side from (3.4.5). This gives

$$\begin{aligned} P_1(f) P_3(v_i^*) - P_3(f) P_1(v_i^*) - \ell \left[P_3(f) P_3(v_i^*) P_1(I_3 \pm I_4) \right. \\ \left. + P_1(f) P_1(v_i^*) P_3(I_1 \pm I_2) \right] = P_1(f_0) P_3(v_i^*) - P_3(f_0) P_1(v_i^*) . \end{aligned}$$

This relation must be valid for arbitrary symmetric v_i and hence

$$P_3(f_0) = P_3(f) + \ell P_1(f) P_3(I_1 \pm I_2) \quad (3.4.10)$$

$$P_1(f_0) = P_1(f) - \ell P_3(f) P_1(I_3 \pm I_4)$$

For if $v_i(k_1 k_2)$ is chosen such that

$$v_i(-k_1, k_2) = v_i(k_1 k_2).$$

Then $P_3(v_i^*) = 0$ and $P_1(v_i^*)$ need not vanish. In this way the first of equations (3.4.10) is obtained and then the second one follows. From

(3.2.18) and (3.2.19) it follows that $C_1 = P_1(f)$ and $D_1 = P_3(f)$.

Solving (3.4.10) for C_1 and D_1 , we obtain the exact values for these constants.

The results for C and D obtained by using Born type trial functions are,

(a) for symmetric solution

$$C_+ = D_+ \frac{P_1(f_0)}{P_3(f_0)} \left[\frac{K_0 - 3B_1}{K_0 - B_1} + \frac{2B_1}{K_0 - B_1} \frac{1}{\Delta_+} \left\{ 1 + \ell P_1(I_3 + I_4) \frac{P_1(f_0)}{P_3(f_0)} \right\} \right]$$

$$D_+ = P_3(f_0) \left[1 + \ell P_3(I_1 + I_2) \frac{P_1(f_0)}{P_3(f_0)} \right]^{-1} \quad (3.4.11)$$

$$\Delta_+ = 1 - \ell \frac{K_0 + B_1}{B_1} \left[P_1(I_3 + I_4) \frac{P_3(f_0)}{P_1(f_0)} + P_3(I_1 + I_2) \frac{P_1(f_0)}{P_3(f_0)} \frac{K_0 - B_1}{K_0 + B_1} \right]$$

where $\ell = 2ATi/4\pi^2$;

(b) for antisymmetric solution

$$C_- = P_1(f_0) \left[1 - \ell P_1(I_3 - I_4) \frac{P_3(f_0)}{P_1(f_0)} \right]^{-1} \quad (3.4.12)$$

$$D_- = C_- \frac{P_3(f_0)}{P_1(f_0)} \left[1 - \frac{\ell}{\Delta_-} \left\{ P_1(I_3 - I_4) \frac{P_3(f_0)}{P_1(f_0)} + P_3(I_1 - I_2) \frac{P_1(f_0)}{P_3(f_0)} \right\} \right] ,$$

$$\Delta_- = 1 - \ell \frac{K_0 + B_1}{2B_1} \left[P_1(I_3 - I_4) \frac{P_3(f_0)}{P_1(f_0)} + P_3(I_1 - I_2) \frac{P_1(f_0)}{P_3(f_0)} \frac{K_0 - B_1}{K_0 + B_1} \right] .$$

If (3.4.11) and (3.4.12) are expanded to the first order in A we obtain,

$$C_{\pm} = P_1(f_0) + \ell P_1(I_3 \pm I_4) P_3(f_0) , \quad (3.4.13)$$

$$D_{\pm} = P_3(f_0) - \ell P_3(I_1 \pm I_2) P_1(f_0) ,$$

where f_0 must be replaced in the above equations by the symmetric or antisymmetric initial state in conformity with the convention on \pm . Comparing (3.4.13) with (3.2.22), (3.2.23), (3.2.25) and (3.2.26), we see that to the first power in A these equations are the same. This is the second Born

approximation and is an instance of the general result obtained in section (2.6) and discussed below equation (2.6.26).

The validity of the expansion which led to (3.4.13) can be investigated for large values of E . The values for the constants become

$$\begin{aligned} C_+ &= (2)^{-1/2} \frac{N\pi}{BT(T+B)} \left(1 - \frac{A}{4\pi} \frac{\pi}{T(T+B)} \right)^{-1}, \\ D_+ &= (2)^{-1/2} \frac{N\pi}{B} \frac{K_0}{K_0^2 + T^2} \left(1 - \frac{A}{4\pi} \frac{\pi}{T(T+B)} \right)^{-1} \end{aligned} \quad (3.4.14)$$

and

$$\begin{aligned} C_- &= -(2)^{-1/2} N\pi / BT(T+B), \\ D_- &= (2)^{-1/2} N\pi K_0 / B(K_0^2 + T^2). \end{aligned} \quad (3.4.15)$$

Comparing these results with the exact values for C and D in the same range of energy values, equation (3.3.14), we find that only if $A/4\pi \ll T(T+B)/\pi$ can the results be said to be in good agreement. In other words the Schwinger variational principle for the Born type trial functions chosen is valid provided the interaction strength A is small and the energy E large. For the calculation of the scattering cross sections in the case of the symmetric solution this result is less satisfactory than the Born result (3.3.15). The antisymmetric solution (3.4.15) is the same as that obtained from the Born approximation, (3.3.15).

Table VI represents the results of the calculations for the scattering cross sections for the values of the parameters $A/4\pi = 1$ and $T = 2B$. The results obtained for the antisymmetrical wave function, Q_{ea} and Q_{ia} , are interesting. Table V shows that for this case the Born approximation gives results in good agreement with the exact ones over the entire energy range. Except for very large values of the energy, the Schwinger variational

principle does not give useful results. Here we have an example of the point stressed in section (2.6). Although there exists values of the energy in which both the Born results and those obtained from the variational principle are in good agreement yet the variational principle fails to extend the usefulness of these results beyond this common domain of applicability. As a matter of fact here the Born approximation is valid over the entire range of the energy.

The results of the calculations for the scattering cross sections, Q_{e_s} and Q_{i_s} , for the symmetric solution are far from satisfactory for both the Born approximation and the Schwinger variational principle. For large values of the energy, the inelastic scattering cross section is sensitive to the values of the constant C whereas the elastic scattering is independent of the values of the constants C and D. This is clear from the expressions for the scattering coefficients given below equation (3.3.14). Therefore the fact, that Q_{i_s} does not approach the exact value for large values of the energy but that the Born result does, implies that the expansion (2.6.25) which relates the Schwinger results to the Born results is invalid and that the condition (2.6.26) is not satisfied. This can be seen in greater detail if equations (3.3.14), (3.3.15) and (3.4.14) are compared. It is then evident that when $A/4\pi \ll T(T+B)/\pi$ that the exact, Born and Schwinger results all agree for large values of E. However, if this relation is not satisfied then the Schwinger results for the scattering cross sections and scattering amplitudes will not be good approximations to the exact values and in fact will give poorer results than the Born results. Using Born trial functions in the Schwinger variational principle gives no assurance of obtaining useful results or even of obtaining an improvement over the Born results.

Table VI

SCHWINGER VARIATIONAL PRINCIPLE

Symmetric Solution			Antisymmetric Solution	
z	Q_{eS}	Q_{iS}	Q_{ea}	Q_{ia}
-.9	6.91562		.875615	
-.5	15.4652		.559420	
-.1	27.5780		.394678	
-.05	29.5696		.379955	
-.01	31.3452		.368888	
-.005	31.4602		.367546	
-.001	31.6319		.366484	
+.001	31.7186	10^{-5} .380808	.365949	10^{-8} .362062
+.005	31.8932	10^{-4} .954174	.364890	10^{-7} .907172
+.01	32.1102	10^{-3} .529686	.363594	10^{-6} .363278
+.05	33.8527	.0139936	.353365	10^{-4} .105366
.1	36.0211	.0569853	.341343	10^{-4} .328266
.5	57.4091	1.65236	.268081	10^{-2} .101452
.9	52.5209	3.86133	.221184	10^{-2} .347454
5.	5.68760	3.56132	.327190	10^{-1} .525699
10.	1.50297	1.85602	.194063	10^{-1} .749875
100.	.0279385	.167764	.0139329	10^{-1} .340824
1000.	10^{-2} .113839	.0192152	.00121054	10^{-2} .426691

z = total energy in units of the bound state energy = E/B^2 .

Q_{eS} = elastic scattering cross section for symmetric solution.

Q_{iS} = inelastic scattering cross section for symmetric solution.

Q_{ea} = elastic scattering cross section for antisymmetric solution.

Q_{ia} = inelastic scattering cross section for antisymmetric solution.

The work in this chapter has elements in common with that of the preceding chapter. The Born expansions in both have been found to converge to the exact solution. For large values of the energy their radii of convergence are also the same. Furthermore the condition $A/4\pi \ll T(T+B)/\pi$ which when satisfied assures good agreement among the exact, Born and Schwinger results for the scattering amplitudes and cross sections is the same in both problems. These similarities impose the same limitations on the approximations as discussed at some length in the preceding chapter. The symmetric problem, however, gives rise to other results. These are best understood in terms of the symmetric and antisymmetric solutions of the problem. Thus the Born expansion for both these solutions converges to the exact solution but have different radii of convergence which approach each other for large values of the energy. The antisymmetric solution, as one would expect on physical grounds, converges more rapidly than the symmetric solution. The Born approximation here in contrast with that for the problem of distinguishable particles has a domain of applicability. This domain is larger for the antisymmetric solution than for the symmetric solution. This is to be expected from the fact that the Born expansion for the former converges much more rapidly than for the latter. The behavior of the Schwinger variational principle when applied to Born type trial functions is such that though the theoretical relation (2.6.25) between the second Born approximation and Schwinger result holds for large values of the total energy in the case of the antisymmetric solution, still the variational principle does not extend the result beyond this common domain. For this same solution the Born approximation gives excellent results throughout the range of energies. One important characteristic of the Born expansion for the symmetric problem with the symmetric perturbation is that the effects due to exchange appear in all terms of the expansion

end in particular in the Born approximation.

The symmetric perturbation considered above is not readily applicable to actual physical problems because it leads to mathematical quantities which are extremely difficult to evaluate. For this reason the problem is usually formulated in terms of an asymmetric perturbation. We now turn to a consideration of this problem described in this way.

Chapter IV

Identical Particles - Asymmetric Perturbation

In general many body problems, for example, the interaction of an electron with a hydrogen atom, are not mathematically tractable when considered from the point of view of the symmetric perturbation. However when these problems are formulated in terms of an asymmetric perturbation the mathematical difficulties are considerably reduced. Since this latter procedure is the one most often found in the literature, it is important to apply it to the problem considered in the previous chapter.

There are some difficulties that center around the calculation of exchange scattering when this problem is treated by approximation methods. For example, there is some question⁴⁰ whether an iterative procedure, the Born expansion, can account for exchange scattering. A method due to Mott and Massey (see footnote 14) which was developed for this purpose has recently been subject to study and criticism^{41,42} (see also footnote 10). Both of these procedures will be studied in some detail. In addition the method given by Borowitz and Friedman (see footnote 10) will be considered. The latter extends the Schwinger variational procedure to three body problems. In what follows, these methods will be studied for their ability to handle exchange scattering.

40. W. Kohn, Private Communication.

41. S. Altshuler, Phys. Rev. 91, 1167 (1953).

42. H. E. Moses, Phys. Rev. 91, 185 (1953).

4.1 An Iterative Procedure

The Schroedinger equation may be written in the following way,

$$\begin{aligned} (k_1^2 + k_2^2 - E)f(k_1 k_2) - \frac{B}{\pi} \int f(k_1 k_2) dk_2 &= \frac{B}{\pi} \int f(k_1 k_2) dk_1 \\ &- \frac{1}{4\pi^2} \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f(k_1' k_2'). \end{aligned} \quad (4.1.1)$$

The left hand side of this equation equated to zero is the unperturbed equation. It represents the physical situation in which particle 2 interacts with the center of force but particle 1 neither interacts with particle 2 nor with the center of force. The solution of the unperturbed equation is

$$f_0(k_1 k_2) = \delta(k_1 - K_0) N / (k_2^2 + B^2), \quad (4.1.2)$$

and describes the initial state of the system in which particle 1 is incident from the left with momentum K_0 and particle 2 is bound.

Equation (4.1.1) is to be solved by inserting (4.1.2) in place of $f(k_1 k_2)$ on the right side of (4.1.1). The solution, $f^{(1)}(k_1 k_2)$, of the resulting equation is then used to replace $f(k_1 k_2)$ on the right hand side of (4.1.1). This determines the function $f^{(2)}(k_1 k_2)$ and the above process can be repeated so that $f^{(n)}(k_1 k_2)$, $n \geq 1$ is a solution of

$$\begin{aligned} (k_1^2 + k_2^2 - E)f^{(n)}(k_1 k_2) - \frac{B}{\pi} \int f^{(n)}(k_1 k_2) dk_2 &= \frac{B}{\pi} \int f^{(n-1)}(k_1 k_2) dk_1 \\ &- \frac{1}{4\pi^2} \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' f^{(n-1)}(k_1' k_2') \end{aligned} \quad (4.1.3)$$

The solution of this equation is (4.1.4)

$$\begin{aligned} f^{(n)}(k_1 k_2) &= f_0(k_1 k_2) + \frac{B}{\pi} \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' f^{(n-1)}(k_1' k_2') \\ &- (2AT1/4\pi^2) \left[P_3(G)P_1(f^{(n-1)}) - P_1(G)P_3(f^{(n-1)}) + P_4(G)P_2(f^{(n-1)}) \right. \\ &\quad \left. - P_2(G)P_4(f^{(n-1)}) \right] \end{aligned}$$

in which the Green's function for the unperturbed equation is used and its explicit form is given by (2.2.37) or (2.2.38). The notation of section (3.2) has been used. Note that $P_i(f^{(n-1)})$, $i = 1, 2, 3, 4$ are constants whereas the terms involving the Green's function are functions of k_1 and k_2 for the integral operators P_i will be understood to operate only on the primed variables of the Green's function.

The evaluation of $P_i(G)$ yields

$$P_1(G) = \frac{1}{k_1^2 + T^2} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} \frac{1}{k_1^2 + k_2^2 - E}, \quad (4.1.5)$$

$$P_2(G) = \left[-\frac{B}{T} \frac{1}{(\sqrt{E - k_1^2} - Bi)(\sqrt{E - k_1^2} + Ti)} + \frac{1}{k_2^2 + T^2} \right] \frac{1}{k_1^2 + k_2^2 - E},$$

$$P_3(G) = \frac{k_1}{(k_1^2 + T^2)} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} \frac{1}{k_1^2 + k_2^2 - E}, \text{ and}$$

$$P_4(G) = \frac{k_2}{k_2^2 + T^2} \frac{1}{k_1^2 + k_2^2 - E}.$$

From equations (4.1.4) and (4.1.5) it is clear that exchange terms can only arise from the second member on the right hand side of (4.1.4). No other member contains a singularity on the real axis of k_2 which at the same time is associated with a bound state in particle 1. The initial state has particle 2 bound and particle 1 incident so that we seek a state in which particle 1 is bound and particle 2 is outgoing. Such a state indicates that particles 1 and 2 have been exchanged. If exchange has taken place it can only arise from the second member, the other members in (4.1.5) do not contain the singularities appropriate for an exchange state. Thus consider

$$\frac{B}{\pi} \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' f^{(n-1)}(k_1' k_2') dk_1' = \quad (4.1.6)$$

$$\frac{B}{\pi} \frac{1}{k_1^2 + k_2^2 - E} \left[\frac{B}{\pi} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} D_1^{(n-1)}(k_1) + D_2^{(n-1)}(k_2) \right],$$

in which

$$D_1^{(n-1)}(k_1) \equiv \int \frac{D_2^{(n-1)}(k_2') dk_2'}{k_1^2 + k_2'^2 - E},$$

and

$$D_2^{(n-1)}(k_2) \equiv \int f^{(n-1)}(k_1 k_2) dk_1 \quad (4.1.7)$$

In (4.1.6) the only term capable of giving rise to the proper singularity on the real axis of k_2 is the term containing $D_2^{(n-1)}(k_2)$.

$$D_2^{(n)}(k_2) = \int dk_1 f^{(n)}(k_1 k_2) \quad (4.1.8)$$

$$\begin{aligned} &= \frac{N}{k_2^2 + B^2} + \frac{Bi}{\sqrt{E - k_2^2}} D_2^{(n-1)}(k_2) - (2ATi/4\pi^2) P^{(n-1)}(k_2) \\ &+ \left(\frac{B}{\pi}\right)^2 \int \frac{dk_1}{k_1^2 + k_2^2 - E} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} D_1^{(n-1)}(k_1), \end{aligned}$$

where

$$\begin{aligned} P^{(n-1)}(k_2) \equiv \int dk_1 \left[P_3(G) P_1(f^{(n-1)}) - P_1(G) P_3(f^{(n-1)}) + P_4(G) P_2(f^{(n-1)}) \right. \\ \left. - P_3(G) P_4(f^{(n-1)}) \right] \end{aligned} \quad (4.1.9)$$

If now we let $n \rightarrow \infty$, then, in an obvious notation,

$$\begin{aligned} D_2(k_2) = \frac{\sqrt{E - k_2^2}}{\sqrt{E - k_2^2} - Bi} \left[\frac{N}{k_2^2 + B^2} + \left(\frac{B}{\pi}\right)^2 \int \frac{dk_1}{k_1^2 + k_2^2 - E} \frac{\sqrt{E - k_1^2}}{\sqrt{E - k_1^2} - Bi} D_1(k_1) \right. \\ \left. - (2ATi/4\pi^2) P(k_2) \right] \end{aligned} \quad (4.1.10)$$

The singularity on the real axis of k_2 is evident in this equation. It is given by the factor outside the square brackets. However this singularity only appears in the limit as $n \rightarrow \infty$. For finite n (4.1.8) does not exhibit this singularity. Hence this iterative procedure when represented by a series does not contain exchange terms. Only when the analytic function represented by the series is determined are the exchange terms properly accounted for.

Equation (4.1.8) may be looked upon as a recurrence relation for $D_2(k_2)$. Employing it in this way we find that the leading term is

$$\frac{N}{k_2^2 + B^2} \left[1 + \frac{B_1}{\sqrt{E - k_2^2}} + \left(\frac{B_1}{\sqrt{E - k_2^2}} \right)^2 + \dots \right] .$$

The series in the brackets is the expansion of

$$\frac{\sqrt{E - k_2^2}}{\sqrt{E - k_2^2} - B_1} = \frac{1}{1 - (B_1/\sqrt{E - k_2^2})}$$

and this expansion is invalid at the singularity, i.e., $k_2^2 = K_0^2$. But this singularity is just the one needed to obtain the scattered wave. This is the reason that the iterative procedure fails to give exchange scattering. The Born expansion breaks down at the singularities of the wave function. The series does not converge to a solution which contains exchange terms.

Let the interaction strength A be set equal to zero. Then the iteration procedure yields

$$\left[\delta(k_1 - K_0) + \frac{B}{\pi} \left\{ 1 + \frac{B_1}{K_0} + \dots + \left(\frac{B_1}{K_0} \right)^n + \right\} \frac{1}{k_1^2 - K_0^2} \right] \frac{N}{k_2^2 + B^2} ,$$

which in the limit as $n \rightarrow \infty$ is

$$\left[\delta(k_1 - K_0) + \frac{B}{\pi} \frac{K_0}{K_0 - Bi} \frac{1}{k_1^2 - K_0^2} \right] \frac{N}{k_2^2 + B^2} .$$

This is the exact solution of the unperturbed symmetrical problem. Not only does the iteration procedure in the limit account for exchange scattering but also gives the correct initial state of the system which is obtained when the problem is considered to be the unperturbed symmetrical one. This latter result is important as we shall see when the Mott and Massey procedure is discussed below.

It must be emphasized that only when the analytic function represented by the series is determined do we get the exact result. Otherwise we obtain an approximation to the exact initial state and exchange scattering is not included.

The Born expansion (3.3.1) obtained from the symmetric perturbation is the result of an iterative procedure similar to the one discussed above. In section (3.3) it was found that the exchange terms were present in all orders of approximation. The reason for this can be found by comparing the Green's functions for these two iterative procedures. In the case of the symmetrical perturbation, the associated Green's function, (3.2.12), contains ab initio all the singularities that contribute to the scattered wave. However when the Green's function (2.2.37) associated with the asymmetrical perturbation is examined we find that not all the singularities of interest are present. Furthermore the use of the initial state in the iterative procedure fails to supply the missing singularities so that if the iterative procedure is to converge to the correct solution it must supply the missing singularities. The individual terms of the

series are free from these singularities. Therefore the sum, i.e., the analytic function represented by the series, must contain them. Mathematically this means that the series is not uniformly convergent.

The iteration procedure evaluated to the second order of approximation yields the following asymptotic part for the approximating wave function,

$$f^{(2)}(k_1 k_2) \sim \delta(k_1 - K_0) N / (k_2^2 + B^2) \quad (4.1.11)$$

$$\begin{aligned} & - \frac{2iAT}{4\pi^2} \frac{N\pi}{B} \left[\frac{C_1 k_1}{k_1^2 + T^2} - \frac{D_1}{K_0^2 + T^2} \left\{ 1 - \frac{B}{T} \left(1 - \frac{iT}{K_0} \right) \right\} \right. \\ & \quad \left. - \frac{D_2}{T(B+T)} \left\{ 1 + \frac{Bi}{K_0} \right\} \right] \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 - K_0^2} \\ & - \frac{2iAT}{4\pi^2} \left[\frac{C_2 k_2 - D_2}{k_2^2 + T^2} \left(1 + \frac{Bi}{|k_1|} \right) + \frac{C_1 k_1 |k_2|}{(k_1^2 + T^2)(|k_2| - Bi)} \right. \\ & \quad \left. - \frac{D_1}{k_1^2 + T^2} \frac{|k_2|}{|k_2| - Bi} \left\{ 1 - \frac{B}{T} \left(1 - \frac{iT}{|k_1|} \right) \right\} \right. \\ & \quad \left. + \frac{BD_2}{T} \frac{|k_2| - iT}{(k_2^2 + T^2)(|k_2| - Bi)} \left(1 + \frac{Bi}{|k_1|} \right) \right] \frac{1}{k_1^2 + k_2^2 - E} . \end{aligned}$$

When this result is compared with the asymptotic part of the exact non-symmetrized solution we find that the exchange term is absent as we expect from the above general discussion but that the other terms in (4.1.11) are the expansion of the exact terms up to the first order in B.

A procedure which takes into account all the singularities of interest will now be considered.

4.2 Mott and Massey Procedure

The Schrodinger equation (3.1.2) is written

(4.2.1)

$$(k_1^2 + k_2^2 - E)f(k_1 k_2) - (B/\pi) \int f(k_1 k_2) dk_2 = \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2')$$

where

$$w(k_1 k_2; k_1' k_2') = (B/\pi) \delta(k_2 - k_2') - (1/4\pi^2) (k_1 k_2 | V | k_1' k_2') . \quad (4.2.2)$$

The unperturbed equation is the left hand side of (4.2.1) set equal to zero. This equation in a slightly different notation has been considered in (2.1) and (2.2). It is separable. Let $f(k_1 k_2) = f_1(k_1) f_2(k_2)$. Then $f_2(k_2)$ must satisfy

$$(k_2^2 - K_2^2) f_2(k_2) - (B/\pi) \int f_2(k_2) dk_2 = 0. \quad (4.2.3)$$

The eigenfunctions of this equation have been found and appear in (2.2.23) and (2.2.6). Explicitly, they are

$$(2 | k_2) \equiv N / (k_2^2 + B^2), \quad N = (2/\pi)^{1/2} B^{3/2}, \quad E = -B^2 \quad (4.2.4)$$

$$(K_2 | k_2) \equiv \delta(k_2 - K_2) + \frac{B}{\pi} \frac{|K_2|}{|K_2| - Bi} \frac{1}{k_2^2 - K_2^2 - i\alpha}; \quad \alpha > 0, \quad E > 0.$$

The orthogonality relations for these eigenfunctions are

$$\int (2 | k_2)^* dk_2 (2 | k_2) = 1. \quad (4.2.5)$$

$$\int (2 | k_2)^* dk_2 (K_2 | k_2) = 0,$$

$$\int (K_2 | k_2)^* dk_2 (K_2 | k_2) = \delta(K_2 - K_2').$$

They also satisfy the closure relation, i.e.,

$$\int (K_2 | k_2')^* dK_2 (K_2 | k_2) + (2 | k_2')^* (2 | k_2) = \delta(k_2 - k_2'). \quad (4.2.6)$$

Therefore these eigenfunctions form a complete set.

The solution $f(k_1 k_2)$ of (4.2.1) considered as a function of k_2 may be expanded in terms of these eigenfunctions.

$$f(k_1 k_2) = f_1(k_1 2)(2|k_2) + \int f_2(k_1 K_2) dK_2 (K_2|k_2), \quad (4.2.7)$$

where $f_1(k_1 2)$ and $f_2(k_1 K_2)$ are the expansion coefficients which are to be determined as functions of k_1 . Insert (4.2.7) into (4.2.1). We obtain

$$\begin{aligned} (k_1^2 - K_0^2) f_1(k_1 2)(2|k_2) + \int (k_1^2 - K_1^2) f_2(k_1 K_2) dK_2 (K_2|k_2) \\ = \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'), \end{aligned} \quad (4.2.8)$$

where $K_0^2 = B^2 + E$ and $K_1^2 = E - K_2^2$. Multiply this equation by $(2|k_2)^* dk_2$ and $(K_2|k_2)^* dk_2$ in turn and integrate over the indicated variable. The following two equations emerge,

$$(k_1^2 - K_0^2) f_1(k_1 2) = \int (2|k_2)^* dk_2 w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'), \quad (4.2.9)$$

and

$$(k_1^2 - K_1^2) f_2(k_1 K_2) = \int (K_2|k_2)^* dk_2 w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'). \quad (4.2.10)$$

The initial state of the system describes particle 1 incident from the left with momentum K_0 and particle 2 bound. Hence the solutions of (4.2.9) and (4.2.10) are

$$f_1(k_1 2) = \delta(k_1 - K_0) + \frac{1}{k_1^2 - K_0^2} \int (2|k_2)^* dk_2 w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'), \quad (4.2.11)$$

and

$$f_2(k_1 K_2) = \frac{1}{k_1^2 - K_1^2} \int (K_2|k_2)^* dk_2 w(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'). \quad (4.2.12)$$

In both of these equations the singularities on the real k_1 axis are explicitly represented. These equations are immediately applicable to the calculation of the elastically and inelastically scattered waves.

An explicit representation of the singularities on the real k_2 axis is desirable. This can be obtained by rewriting equation (4.2.1) as follows,

$$(k_1^2 + k_2^2 - E)f(k_1 k_2) - (B/\pi) \int f(k_1 k_2) dk_1 = \int v(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2') \quad (4.2.13)$$

where

$$v(k_1 k_2; k_1' k_2') = (B/\pi) \delta(k_1 - k_1') - (1/4\pi^2) (k_1 k_2 | \nabla | k_1' k_2'). \quad (4.2.14)$$

The left hand side of (4.2.13) equated to zero is now considered. It is treated in a manner completely analogous to that given equation (4.2.3). The complete set of eigenfunctions which are obtained are,

$$(1|k_1) \equiv N/(k_1^2 + B^2); \quad N = (2/\pi)^{1/2} B^{3/2} \quad (4.2.15)$$

$$(K_1|k_1) \equiv \delta(k_1 - K_1) + \frac{B}{\pi} \frac{|K_1|}{|K_1| - B^2} \frac{1}{k_1^2 - K_1^2 - i\alpha}; \quad \alpha > 0$$

These eigenfunctions satisfy similar orthogonality and closure relations as do the eigenfunctions (4.2.4) and form a complete set for functions which depend on k_1 .

Consider the solution $f(k_1 k_2)$ of (4.2.1) as a function of k_1 and expand it in terms of the above eigenfunctions. Then

$$f(k_1 k_2) = g_1(1k_2)(1|k_1) + \int g_2(K_1 k_2) dK_1 (K_1|k_1), \quad (4.2.16)$$

in which $g_1(1k_2)$ and $g_2(K_1 k_2)$ are the coefficients of the expansion and are functions of k_2 which are to be determined. Following the procedure used in the evaluation of $f_1(k_1 k_2)$ and $f_2(k_1 k_2)$, we find that

$$g_1(1k_2) = \frac{1}{k_2^2 - K_0^2} \int (1|k_1)^* dk_1 v(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'), \quad (4.2.17)$$

and

$$g_2(K_1 k_2) = \frac{1}{k_2^2 - K_2^2} \int (K_1|k_1)^* dk_1 v(k_1 k_2; k_1' k_2') dk_1' dk_2' f(k_1' k_2'). \quad (4.2.18)$$

Here $K_2^2 = E - K_1^2$ and $K_0^2 = B^2 + E$. These equations do not contain any inhomogeneous terms since the physical situation requires that particles 2 must be outgoing. In these equations the explicit dependence $f(k_1 k_2)$ on the singularities on the real axis of k_2 is exhibited.

Equations (4.2.11), (4.2.12), (4.2.17) and (4.2.18) are exact. To solve them approximately, $f(k_1 k_2)$ in the integrands on the right hand side of these equations is replaced by the initial state of the system which is given by

$$f_0(k_1 k_2) = \delta(k_1 - K_0) N / (k_2^2 + B^2) \quad (4.2.19)$$

The results of the calculations are

$$f_1(k_1 k_2) = \delta(k_1 - K_0) + \frac{1}{k_1^2 - K_0^2} \left[\frac{B}{\pi} - \ell \left(\frac{N\pi}{B} \right)^2 \frac{k_1 - K_0}{(k_1^2 + T^2)(K_0^2 + T^2)} \right], \quad (4.2.20)$$

and

$$g_1(1k_2) = \frac{1}{k_2^2 - K_0^2} \left[\frac{N^2}{K_0^2 + B^2} - \ell \left(\frac{N\pi}{B} \right)^2 \frac{1}{T(T+B)} \left\{ \frac{k_2}{k_2^2 + T^2} - \frac{K_0}{K_0^2 + T^2} \right\} \right]. \quad (4.2.21)$$

The terms $f_2(k_1 K_2)$ and $g_2(K_1 k_2)$ are not considered since these terms give the contributions to the inelastically scattered waves.

The exchange scattering terms are given by (4.2.21). Both equations give the asymptotic part of $f(k_1 k_2)$; (4.2.20) for the singularities on the real axis of k_1 and (4.2.21) for those on the real axis of k_2 . Combining these results we find that the elastic scattering amplitudes for the symmetrized solutions are

$$(2)^{-1/2} \left[\frac{B}{\pi} \pm \frac{N^2}{K_o^2 + B^2} - \ell \left(\frac{N\pi}{B} \right)^2 \frac{k_1 - K_o}{(K_o^2 + T^2)} \frac{1}{T(T+B)} \left\{ \frac{T(T+B)}{K_o^2 + T^2} \pm 1 \right\} \right]. \quad (4.2.22)$$

Except for the term $N^2/(K_o^2 + B^2)$ this expression is an approximation to the elastic scattering amplitude of the exact solution in which $K_o/(K_o - Bi)$ is replaced by unity (valid for K_o and hence E large), and the constants C and D are replaced by the values obtained for them by the Born approximation in the symmetric perturbation formulation of this problem.

The term $N^2/(K_o^2 + B^2)$ which appears in (4.2.22) is disconcerting. It occurs in (4.2.21) and implies that exchange scattering takes place even if the interaction between the particles vanishes, for when $A = 0$, $g_1(k_2)$ does not vanish. On physical grounds there cannot be exchange scattering when the particles fail to interact.

Equation (4.2.21) is admittedly the result of using an approximation to the exact wave function. If we assume A to be zero and iterate using $f(k_1 k_2)$ determined by (4.2.17), (4.2.18) and $f_o(k_1 k_2)$, we find that the n^{th} iteration gives

$$\varepsilon_1^{(n)}(k_2) = \left(\frac{Bi}{K_o} \right)^n \frac{N^2}{K_o^2 + B^2} \frac{1}{k_2^2 - K_o^2}, \quad (4.2.23)$$

and

$$\varepsilon_2^{(n)}(k_1 k_2) = \left(\frac{Bi}{|K_2|} \right)^n N(K_1 | K_o)^* \frac{1}{k_2^2 - K_2^2}.$$

These expressions converge to zero for $|Bi/K_o| < 1$ and $|Bi/K_2| < 1$.

For real values of K_o and K_2 other than those satisfying these inequalities these expressions diverge. Thus the physically acceptable solutions vanish as $n \rightarrow \infty$. The contributions to exchange scattering given by $\pm N^2/(K_o^2 + B^2)$ in the first approximation is spurious.

The exact mathematical calculations justify the physical requirements.

Practically, however, the calculations are restricted to first, second or

possibly third order approximations. In this situation the contributions to the scattering from the spurious terms assume an unwarranted importance. The difficulty arises from the use of the initial state as a first approximation to the exact solution. The physical basis for taking the initial state as a first order approximation is that for energies sufficiently large it is expected that the interaction of the incident particle with the atom will have a negligible effect on the initial state of the system. When exchange phenomena are possible this assumption is incorrect. For exchange phenomena to occur two conditions must be met. First, the incident particle must interact with the center of force so that it can be bound and secondly, it must interact with the bound particle so that an energy transfer is possible. When approximation methods are to be used, the relative order of magnitude of these interactions is also important. Naive considerations lead us to expect that the interaction between the incident and bound particles is smaller on the average than the interaction between the incident particle and the center of force. Consider the problem in which electrons are incident on hydrogen atoms. The distortion of the bound electronic charge by the incident electrons would on the average result in the distance between the electrons being larger than that between the nucleus and incident electrons. Furthermore the fact that the incident electron can be bound implies that the attractive forces which exist would result in the enhancement of the distortion of the electronic cloud about the nucleus and thus increase the influence of the nucleus on the incident electrons. Hence a first order approximation which takes into account the relative magnitudes of the interactions involved is one which contains the effect of the interaction of the center of force on the incident particles.

The above physical argument can be reinforced by considering equations (4.2.11) and (4.2.17). In (4.2.11) replace $f(k_1 k_2)$ with its expansion (4.2.7). Then

$$f_1(k_1^2) = \delta(k_1 - K_0) + \frac{B}{\pi} \frac{1}{k_1^2 - K_0^2} \int f_1(k_1^2) dk_1 \quad (4.2.24)$$

$$- \frac{1}{4\pi^2} \frac{1}{k_1^2 - K_0^2} \int (2|k_2)^* dk_2 (k_1 k_2 | V | k_1^! k_2^!) dk_1^! dk_2^! f(k_1^! k_2^!).$$

The first two terms on the right, since $\int f_1(k_1^2) dk_1$ is a constant, have the form of $(K_0 | k_1)$ which is a solution of the unperturbed equation that takes into account the interaction of the incident particle with the center of force. Now take $(K_0 | k_1)(2|k_2)$ as the first order approximation to $f(k_1 k_2)$ and insert it into (4.2.17). We obtain

$$g_1(1k_2) = - \frac{1}{4\pi^2} \frac{1}{k_2^2 - K_0^2} \int (1|k_1)^* dk_1 (k_1 k_2 | V | k_1^! k_2^!) dk_1^! dk_2^! (K_0 | k_1^!)(2|k_2^!). \quad (4.2.25)$$

Here we see that the exchange scattering vanishes when the interaction between the incident and bound particles vanish. The result of using an approximating function of the type considered has been to eliminate the spurious terms previously obtained in (4.2.21) and to make $g_1(1k_2)$ of (4.2.25) depend on the interaction between the incident and bound particles only. The interaction between the incident particle and the center of force has been incorporated in the trial function used. In this way the order of magnitude of the two interactions has been properly treated and the weaker interaction is now the perturbation.

A detailed calculation using the trial function $(K_0 | k_1)(2|k_2)$ gives the following asymptotic part for the elastic scattering coefficient for the symmetric and antisymmetric wave functions,

(4.2.26)

$$(2)^{-1/2} \left[\frac{B}{\pi} \frac{K_0}{K_0 - B i} - \ell \left(\frac{N\pi}{B} \right)^2 \left\{ \frac{k_1}{K_0^2 + T^2} \left(\frac{T-B}{T} \frac{1}{K_0^2 + T^2} \pm \frac{1}{T(T+B)} \right) \frac{K_0}{K_0 - B i} \right. \right. \\ \left. \left. - \frac{K_0}{K_0^2 + T^2} \frac{1}{T(T+B)} \left(\frac{T(T+B)}{K_0^2 + T^2} \pm 1 \right) \right\} \right]$$

If this result is compared with (4.2.22), which was obtained by using the initial state as a first order approximation to the exact solution, we find that the spurious term is absent and that the factor $K_0/(K_0 - B i)$ appears instead of its approximation by unity. Furthermore the constants C and D are much better approximated by (4.2.26) than by (4.2.22). Equation (4.2.26) is except for the last term in the curly brackets identical to the result obtained by the Born approximation in section (3.3). This is significant because the Born approximation in that section is the leading term in the Born expansion which is known to converge. Thus the Mott and Massey procedure with trial functions which take into account the effect of the interaction between the incident particles and the center of force will yield results comparable to those obtained by treating the problem by the much more mathematically difficult symmetric perturbation procedure.

There is yet another argument from the computer's point of view for the use of the altered initial state trial functions discussed above. Namely, if the interaction term were to be neglected both representations (4.2.11) and (4.2.16) of the exact solutions must give the initial state of the system. This is easily verified to be so. But if the procedure leads to this result which can be obtained exactly, surely an approximation method should avail itself of this fact from the start.

The above discussion is not restricted to the problem under

consideration but carries over directly to actual physical problems. The physical arguments are of general applicability and we have applied them to this problem so that they could be illustrated and examined in detail.

Table VII lists the numerical results obtained for the elastic and inelastic scattering cross sections from the Mott and Massey procedure. The first two columns were obtained for the symmetric solution, and the last two for the antisymmetric solution. The column headed Q_{eB} is the elastic scattering cross section obtained with the initial state of the system taken as the approximation to the exact solution and Q_{eM} heads the column for which the altered initial state, i.e., the state which takes into account the effect of the center of force, was used as an approximation to the exact wave function.

The first two columns give exceedingly poor approximations as comparison with Table IV will show except for large values of E . This is expected since for the symmetric solution we have already seen that the Born approximation with the symmetric perturbation is unsatisfactory for all but large values of E and the results here are approximations to this approximation.

The last two columns when compared with Table V indicates that Q_{eM} is a much better approximation than Q_{eS} . Here the comparison is much more significant than the previous one. For the Born approximation with the symmetric perturbation for the antisymmetric wave function yields excellent values for the scattering cross sections as Table V indicates. As a matter of fact the Born approximation is part of the Born expansion and this is well within its radius of convergence as is also shown in Table V. The Q_{eM} and Q_{eB} of Table VII are approximations to the Q_{eB} of Table V as was shown in equations (4.2.22) and (4.2.26) and the fact that Q_{eM} is

Table VII

z	Symmetric Solution		Antisymmetric Solution	
	Q_{eB}	Q_{eM}	Q_{eB}	Q_{eM}
-.9	80.6882	155.576	7.14250	8.84130
-.5	20.3238	76.0175	.414772	3.05059
-.1	11.9145	43.5778	10^{-1} .767417	1.33780
-.05	11.3275	41.1821	10^{-1} .651345	1.22707
-.01	10.9017	39.3207	10^{-1} .577614	1.14778
-.005	10.8451	38.8173	10^{-1} .569441	1.13846
-.001	10.8040	38.6335	10^{-1} .561920	1.13105
+.001	10.7836	38.5421	10^{-1} .559906	1.12737
+.005	10.7493	38.3599	10^{-1} .553718	1.12005
+.01	10.6927	38.1334	10^{-1} .546157	1.11102
+.05	10.3053	36.3899	10^{-1} .492562	1.04245
+.1	9.85636	34.3628	10^{-1} .440770	.965360
+.5	7.23167	22.6594	10^{-1} .362542	.579865
+.9	5.60363	15.8669	10^{-1} .509812	.409900
5.	1.17386	1.99032	.141181	.184651
10.	.429427	.560365	.119278	.125789
100.	10^{-1} .138501	10^{-1} .143099	10^{-1} .123460	10^{-1} .114606
1000.	10^{-2} .103816	10^{-2} .104165	10^{-2} .102935	10^{-2} .101717

superior to Q_{eB} confirms what has been said about the altered initial state as an approximation to the exact wave function.

As in previous considerations, it is desirable to study the Schwinger variational principle.

4.3 The Schwinger Variational Principle—Borowitz-Friedman Procedure

The solution of the Schroedinger equation (3.1.2) is written as a sum of the incident wave and an outgoing wave. Thus

$$f(k_1 k_2) = f_0(k_1 k_2) + h(k_1 k_2) \quad (4.3.1)$$

where $f_0(k_1 k_2)$ is the solution of the unperturbed equation and is given by (4.2.19). The function $h(k_1 k_2)$ represents the outgoing particles 1 and 2. The Borowitz-Friedman (see footnote 10) procedure constructs an integral equation for $h(k_1 k_2)$ from which the exchange scattering amplitudes may be computed by means of the Schwinger variational principle. This procedure can be formulated so that the direct as well as the exchange scattering amplitudes can be treated symmetrically.

Substitute (4.3.1) into the Schroedinger equation (3.1.2). Then $h(k_1 k_2)$ must satisfy

$$\begin{aligned} (k_1^2 + k_2^2 - E)h(k_1 k_2) - (B/\pi) \int h(k_1 k_2) dk_1 - (B/\pi) \int h(k_1 k_2) dk_2 \\ - (B/\pi) \int f_0(k_1 k_2) dk_1 + (1/4\pi^2) \int (k_1 k_2 | V | k_1' k_2') dk_1' dk_2' \left[f_0(k_1' k_2') + h(k_1' k_2') \right] = 0 \end{aligned} \quad (4.3.2)$$

This equation may be written in the following two ways

$$\begin{aligned} (k_1^2 + k_2^2 - E)h(k_1 k_2) - (B/\pi) \int h(k_1 k_2) dk_1 = \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' f_0(k_1' k_2') \\ + \int v(k_1 k_2; k_1' k_2') dk_1' dk_2' h(k_1' k_2'), \end{aligned} \quad (4.3.3)$$

or (4.3.4)

$$(k_1^2 + k_2^2 - E)h(k_1 k_2) - (B/\pi) \int h(k_1 k_2) dk_2 = \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' f_0(k_1' k_2') \\ + \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' h(k_1' k_2'),$$

in which

$$w(k_1 k_2; k_1' k_2') \equiv (B/\pi) \delta(k_2 - k_2') - (1/4\pi^2) (k_1 k_2 | V | k_1' k_2') \quad (4.3.5)$$

and

$$v(k_1 k_2; k_1' k_2') \equiv (B/\pi) \delta(k_1 - k_1') - (1/4\pi^2) (k_1 k_2 | V | k_1' k_2'). \quad (4.3.6)$$

Note that

$$w(k_1 k_2; k_1' k_2') = v(k_2 k_1; k_2' k_1'). \quad (4.3.7)$$

Denote the Green's functions of the left hand sides of (4.3.3) and (4.3.4) by $G^{(1)}(k_1 k_2; k_1' k_2')$ and $G(k_1 k_2; k_1' k_2')$ respectively. The relation between these Green's functions is

$$G^{(1)}(k_1 k_2; k_1' k_2') = G(k_2 k_1; k_2' k_1'). \quad (4.3.8)$$

This follows from the fact that the left hand sides of equations (4.3.3) and (4.3.4) differ only in an interchange of k_1 and k_2 . The explicit expression for $G(k_1 k_2; k_1' k_2')$ is given by (2.2.37) or (2.2.38).

We may now represent $h(k_1 k_2)$ by either of the following two integral equations:

$$h(k_1 k_2) = \alpha(k_1 k_2) + \int G^{(1)}(k_1 k_2; k_1' k_2') dk_1' dk_2' v(k_1' k_2'; k_1'' k_2'') dk_1'' dk_2'' h(k_1'' k_2'') \quad (4.3.9)$$

or (4.3.10)

$$h(k_1 k_2) = \beta(k_1 k_2) + \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' w(k_1' k_2'; k_1'' k_2'') dk_1'' dk_2'' h(k_1'' k_2''),$$

where (4.3.11)

$$\alpha(k_1 k_2) = \int G^{(1)}(k_1 k_2; k_1' k_2') dk_1' dk_2' w(k_1' k_2'; k_1'' k_2'') dk_1'' dk_2'' f_0(k_1'' k_2''),$$

and

(4.3.12)

$$\beta(k_1 k_2) = \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' w(k_1' k_2'; k_1'' k_2'') dk_1'' dk_2'' f_0(k_1'' k_2'').$$

The integral equation which represents the solution of (3.1.2) is

(4.3.13)

$$f(k_1 k_2) = f_0(k_1 k_2) + \int G(k_1 k_2; k_1' k_2') dk_1' dk_2' w(k_1' k_2'; k_1'' k_2'') dk_1'' dk_2'' f(k_1'' k_2'').$$

When $f_0(k_1 k_2)$ is substituted for $f(k_1 k_2)$ in the above integral then the resulting integral is $\beta(k_1 k_2)$. Hence $\beta(k_1 k_2)$ is the correction to the initial state that is obtained from the Born approximation. The expression $\alpha(k_1 k_2)$ cannot be similarly interpreted.

The integral equations (4.3.9) and (4.3.10) have the property of explicitly expressing the asymptotic part of $h(k_1 k_2)$ in the momenta k_2 and k_1 respectively. This is due to the fact that the respective Green's functions are explicitly given at the singularities on the real axis of k_2 and k_1 respectively.

Equation (4.3.9) which expresses the asymptotic part of $h(k_1 k_2)$ on the real axis of k_2 explicitly does not vanish with the interaction between the incident and bound particles. This is as it should be for the equation represents a solution of the problem and when the interaction vanishes there are still outgoing waves, namely, those waves that result from the interaction between the incident waves and the center of force. It is easily verified that with the interaction between the incident and bound particles set equal to zero that

(4.3.14)

$$h(k_1 k_2) = \frac{B}{\pi} \frac{K_0}{K_0 - B i} \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 - K_0^2}.$$

With this expression inserted in (4.3.1) we indeed obtain the solution of the unperturbed problem. This result implies that $h(k_1 k_2)$ must not be set equal to zero on the right side of (4.3.9), for then in this approximation with the interaction between incident and bound particles set equal to zero, we obtain

$$h(k_1 k_2) = \frac{B}{\pi} \frac{(E - k_2^2)^{1/2}}{(E - k_2^2)^{1/2} - B i} \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 + k_2^2 - E}$$

which has for its asymptotic part

$$h(k_1 k_2) \sim \frac{N^2}{k_0^2 + B^2} \frac{N}{k_1^2 + B^2} \frac{1}{k_2^2 - k_0^2} + \frac{B}{\pi} \frac{|k_1|}{|k_1| - B i} \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 + k_2^2 - E}.$$

This last expression indicates that there is exchange scattering even though physically we know this to be impossible. The contribution to exchange scattering is just the spurious term found in the preceding section. Secondly, trial functions for $h(k_1 k_2)$ must be chosen such that it consists of the term (4.3.11) plus a function that depends on the interaction between the incident and bound particles. Such a choice not only describes what is occurring physically but also insures that exchange scattering will vanish when the interaction does. The need to choose $h(k_1 k_2)$ in this way is a confirmation of the analysis of this problem given in the preceding section.

The asymptotic part of $\beta(k_1 k_2)$ which is independent of the interaction between the incident and bound particles is

$$\frac{B}{\pi} \frac{N}{k_2^2 + B^2} \frac{1}{k_1^2 - k_0^2}.$$

Except for a constant factor, this expression is the same as (4.3.14). Thus $\beta(k_1 k_2)$ has just the form necessary to serve as a trial function for $h(k_1 k_2)$. Calculations have been carried out using (4.3.14) as an approximation to the exact solution. The results are identical to (4.2.26) which was obtained from the Mott and Massey procedure with the altered initial state as the trial function. This is to be expected. (See footnote 10). But now the integral equations are in such a form that we can

apply the Schwinger variational principle to them.

The integral equations (4.3.9) and (4.3.10) may be written

$$a(k_1 k_2) = K h(k_1' k_2'), \quad (4.3.15)$$

and

$$a'(k_1 k_2) = L h(k_1' k_2') \quad (4.3.16)$$

respectively, where

$$a(k_1 k_2) = \int v(k_1 k_2; k_1' k_2') dk_1' dk_2' \alpha(k_1' k_2') \quad (4.3.17)$$

$$a'(k_1 k_2) = \int w(k_1 k_2; k_1' k_2') dk_1' dk_2' \beta(k_1' k_2'), \quad (4.3.18)$$

and K and L are integral operators with kernels

$$(4.3.19)$$

$$K(k_1 k_2; k_1' k_2') = \int \left[\delta(k_1 - k_1''') \delta(k_2 - k_2''') v(k_1 k_2; k_1'' k_2'') dk_1'' dk_2'' G^{(1)}(k_1'' k_2''; k_1''' k_2''') \right] \\ \cdot dk_1''' dk_2''' v(k_1''' k_2'''; k_1' k_2'),$$

and

$$(4.3.20)$$

$$L(k_1 k_2; k_1' k_2') = \int \left[\delta(k_1 - k_1''') \delta(k_2 - k_2''') w(k_1 k_2; k_1'' k_2'') dk_1'' dk_2'' G(k_1'' k_2''; k_1''' k_2''') \right] \\ \cdot dk_1''' dk_2''' w(k_1''' k_2'''; k_1' k_2').$$

Each of the equations (4.3.15) and (4.3.16) can be treated in a manner completely analogous to the development of similar equations in section (2.6). This variational principle has been exhaustively discussed in Chapters II and III. We shall not repeat the details here except to say that the computations have been carried out only for the determination of the direct and exchange scattering amplitudes. From these we obtained the scattering cross sections by pursuing the procedure used in calculating the exact cross sections in section (2.3).

Table VIII

SCHWINGER VARIATIONAL PRINCIPLE
BOROWITZ-FRIEDMAN

	Symmetric	Antisymmetric
	Q_{es}	Q_{ea}
-.9	89.8027	6.83310
-.5	19.6501	.195340
-.1	12.0166	10^{-1} .197900
-.05	11.4933	10^{-1} .204200
-.01	11.1119	10^{-1} .206700
-.005	11.0686	10^{-1} .208400
-.001	11.0324	10^{-1} .208900
+.001	11.0164	10^{-1} .209600
+.005	10.9796	10^{-1} .214300
+.01	10.9420	10^{-1} .214300
+.05	10.6158	10^{-1} .302700
+.1	10.2279	10^{-1} .263500
+.5	7.91153	10^{-1} .717500
+.9	6.40569	.124870
5.	1.36008	.205875
10.	.467606	.151366
100.	10^{-1} .137221	10^{-1} .126091
1000.	10^{-2} .104397	10^{-2} .102327

Table VIII contains the results of the numerical calculations. Here again we find that for the Born trial function the results are far from satisfactory. This failure is due to the fact that in this case (2.6.26) holds for the symmetrical and antisymmetrical solutions only for large E . The variational principle does not extend the usefulness of the results to smaller values of E . This difficulty has been met with before.

To recapitulate: The application of the iterative procedure—the Born expansion—leads to results which differ from those obtained in Chapters II and III. The series representation of the solution does not converge to a solution which accounts for exchange scattering. Therefore this iterative procedure cannot yield any information about exchange scattering. The Mott and Massey procedure does, however, give exchange scattering. But if the initial state is used as a first order approximation to the solution, spurious terms are obtained. If the initial state is altered by including the effect of the interaction of the center of force on the incident particles (the altered initial state is to consist of incident waves plus outgoing spherical waves and is a solution of the unperturbed wave equation in which the interaction between incident and bound particles is set equal to zero), then the spurious terms do not appear and in addition the approximation to exchange scattering is improved. These results are directly applicable to actual physical problems. The Borowitz-Friedman approach to this problem is to construct integral equations for the scattered wave only. In this formulation an iterative procedure is possible for the calculation of the exchanged scattered wave. This is not true of the Mott and Massey (see footnote 10) procedure. Moreover the analysis of this procedure confirms the advisability of using the altered initial state as a trial function. In addition this method can make use of the Schwinger variational principle for the calculation of the exchange scattered amplitudes which is not a property of the Mott and Massey

formulation of the problem. The application of the Schwinger variational principle leads to results which have already been noted in the preceding chapters.

Chapter V

CONCLUDING REMARKS

In the preceding chapters, we have considered the Born approximation with the associated Born expansion, the Schwinger and Hulthén-Kohn variational principles, and where occasions required it, some variations of these approximation methods such as the Mott and Massey procedure and the Borowitz-Friedman extension of the Schwinger variational principle. These methods have been applied to specific problems with defined interactions and the conclusions which were reached must now be examined in the light of their general applicability.

Specific problems serve at least three important purposes. First, they may be counter examples to conjectures, to seemingly plausible assumptions or to conclusions which have been extrapolated from known results. Secondly, they can suggest ways and means of obtaining general results. Finally, they may point out certain aspects of general significance which are worth further investigation. The problems studied here have been fruitful in these respects.

Consider the Born expansion which incorporates the Born approximation and which was studied in Chapters II and III. It was shown that the Born expansion converged to the exact solutions. In the first of the problems, dealt with in Chapter II, the Born approximation does not have any useful domain of applicability whatever the value of the total energy unless the interaction between the incident and bound particles is very weak. Here the meaning of weak is related to the shortness of the range of the interaction. That the Born approximation may not have a useful domain of applicability is not a consequence solely of the interaction employed in this problem.

Jost and Pais (see footnote 5) obtain a similar result in an analysis of the Born approximation for a Yukawa potential. Furthermore there is an additional result that their problem has in common with the one studied here which is that the second Born approximation furnishes a substantial correction to the Born approximation even for extremely large values of the energy. For the problem dealt with here this substantial correction defines a useful domain of applicability for the results so obtained. Moreover, this example indicates that in general the second Born approximation must be calculated if useful results are to be obtained. Physically the need for such additional calculation can be understood qualitatively by considering the Born expansion of the exact solution which may be represented in general by

$$f = f_0 + \sum_{n=1}^{\infty} f_n = f_0 + g, \quad (5.1)$$

where f is the exact solution, f_0 the initial state of the system and $g \equiv \sum f_n$ represents the scattered wave. Here the Born approximation is given by $f_0 + f_1$ and the second Born approximation by $f_0 + f_1 + f_2$. The initial state of the system, f_0 , does not depend on the interaction which is taken as the perturbation. However, the scattered wave, g , does. Calculating the Born approximation, $f_0 + f_1$ yields the first term in the expansion for g which of course contains no information about the usefulness of this expansion for g though it does furnish a measure of the effect of the perturbation on the initial state. But for the Born approximation to be of use the effect of the perturbation on the successive terms of the expansion for g must be determined and this involves at least a calculation of the second Born approximation and a comparison of this with the Born approximation. Dalitz (see footnote 5) in a study of the Yukawa potential

in the limit as it approaches the Coulomb potential also found it necessary to go beyond the Born approximation. Actually he calculated terms of the third order in the Born expansion although the second order terms already furnish information about the convergence of the series.

The calculation of higher order terms in the Born expansion is difficult. Thus we have considered the Schwinger variational principle restricted in application to Born trial fields because otherwise the mathematical computations become extremely complicated. However, for such trial functions we find that the relation of the second Born to Born approximation discussed above again plays a significant role. In Chapter II it was shown that if

$$\left| (f_{01}, VGVf_0) / (f_{01}, Vf_0) \right| < 1 \quad (5.2)$$

then the variational results include the second Born approximation. The numerator of this ratio is the asymptotic part of f_2 and the denominator is the asymptotic part of f_1 both of which appear in the expansion (5.1). For the problem considered in Chapter II, the second Born approximation is useful for all values of the interaction strength A . However, in this case (5.2) is not satisfied unless the values of A are restricted. Thus we see that the variational results do not include the second Born approximation which is known to be good unless the interaction is weak and weak here means that the Born approximation is good. Obviously under these conditions there is no point in using a variational principle. In Chapter III the situation is different. Both the variational and Born results for the antisymmetric solution are good approximations to the exact values for large values of the energy. But as the energy becomes smaller the variational results get poorer whereas the Born results are good throughout the energy range. Here it is clear that the variational principle fails to extend the Born results beyond their common domain of agreement. Although the variational and Born results may not be good approximations to the

exact values for large values of the energy yet, as an example in Chapter II reveals, the variational results may be in good agreement with the exact values for small energies where the Born results are inadequate. From these results enumerated above, it is clear that the Schwinger variational principle restricted in application to Born trial functions does not necessarily yield results superior to the Born or second Born approximation. The basic problem here is the determination of some guide for the selection of appropriate trial functions. We will return to this point after a consideration of the Hulthén-Kohn variational procedure.

This variational procedure is more amenable to mathematical calculation than the Schwinger variational principle because it is not formulated in terms of a Green's function. For comparison purposes its application in the preceding chapter was restricted to Born trial functions but then the results so obtained were shown to be equivalent to the Born results. Though the mathematical simplicity of the Hulthén-Kohn variational principle was not fully exploited yet a general relation between this principle and Schwinger's was established. The significance of this relationship is due to the fact that Kato (see footnote 9), for two body problems, has been able to establish upper and lower bounds for the Schwinger and Hulthén-Kohn variational principles. This was accomplished by suitably restricting the class of trial functions to be used. The general relationship between these principles and the relative mathematical simplicity of the Hulthén-Kohn variational principle indicates the possibility of extending Kato's result to many body problems in terms of trial functions to which the Hulthén-Kohn variational principle may be directly applied.

Chapter IV dealt with the problem of exchange scattering. The formulation of the symmetric problem using a symmetric perturbation led to the result that each term in the Born expansion gave evidence of exchange scattering and in particular the Born approximation takes this effect into

account. This same problem using an asymmetric perturbation leads to difficulties in the calculation of exchange scattering. The Born expansion, in this case, gave rise to a series representation of the exact solution which did not contain exchange scattering. This is due to the fact that the series is not valid at the singularity of the wave function which yields the exchange scattered wave. This behavior illustrates and supports a conjecture due to Kohn (see footnote 40) in which it is stated that the Born expansion does not converge to a solution which accounts for exchange scattering. The latter physical process, of course, must be possible for the problem. Though this conjecture has been verified only for the specific problem considered here, yet the result throws considerable doubt on the applicability of this iterative procedure to a determination of exchange scattering in actual physical problems. The Mott and Massey procedure which was developed to handle this problem, in turn, gave rise to difficulties which have only recently (see footnotes 40,41) been cleared up. In Chapter IV this procedure is examined when the Born approximating procedure is used, i.e., the initial state is used as a first order approximation to the exact function. The result of this study was that this method does account for exchange scattering but that spurious terms arise in the calculation of the exchange scattered wave. These spurious terms assume unwarranted importance especially if the calculated approximation is used in an iterative procedure. However, if the initial state is altered so that the effect of the interaction between the incident particles and the center of force is taken into account (describing this in coordinate space, the altered initial state is the incident wave plus outgoing spherical waves), then no spurious terms arise and the approximation so obtained is comparable to the Born approximation for the problem formulated with a symmetric perturbation. These results are of general validity and are not restricted to the particular problems considered here.

APPENDIX I

The explicit expressions for the quantities appearing in equations (2.2.16), (2.2.17), and (2.2.18) are

$$J_1 = \int \frac{dk_1}{(k_1 + iT)(P - B1)(P + iT)} \quad ; \quad P = (E - k_1^2)^{1/2}$$

$$= - \frac{i}{B+T} \left[\frac{1}{K_0^2 + T^2} \left\{ \pi B - \frac{BT1}{K_0} (\pi + i \ln S(B)) - i(T^2 + E)^{1/2} (\pi - i \ln S(T)) \right\} \right.$$

$$\left. + \frac{1}{2T^2 + E} \left\{ \pi T + \frac{E1}{(T^2 + E)^{1/2}} (\pi - i \ln S(T)) \right\} \right] .$$

$$J_2 = \int \frac{dk_1}{P(P - B1)(P + iT)^2}$$

$$= \frac{2}{(B+T)(T^2 + E)} + \frac{1}{K_0(B+T)^2} (\pi + i \ln S(B)) - \frac{i(\pi - \ln S(T))}{(B+T)(T^2 + E)^{1/2}} \left(\frac{1}{B+T} + \frac{T}{T^2 + E} \right)$$

$$J_3 = \int \frac{dk_1}{P(k_1^2 + T^2)} = \frac{1}{T(T^2 + E)^{1/2}} (\pi - i \ln S(T)) .$$

$$J_4 = \int \frac{dk_1}{(k_1 + iT)(P - B1)}$$

$$= \frac{1}{K_0^2 + T^2} \left[\pi B - \frac{BT1}{K_0} (\pi + i \ln S(B)) - i(T^2 + E)^{1/2} (\pi - i \ln S(T)) \right]$$

$$S(x) = \left\{ (x^2 + E)^{1/2} + x \right\} / \left\{ (x^2 + E)^{1/2} - x \right\} .$$

In the above expressions $E > 0$. For $E < 0$ the logarithmic terms are defined by

$$\ln S(x) = \ln \left\{ (x^2 + E)^{1/2} + x \right\} - \ln \left\{ (x^2 + E)^{1/2} - x \right\}$$

where for each term the principal values of the logarithms are to be taken.

For very large positive values of E, we find that

$$J_1 \sim \pi(B - 2T) (E)^{-3/2} - \pi(E)^{-1} i$$

$$J_2 \sim (4/3) (B - 2T) E^{-2} - (\pi/2) E^{-3/2} i$$

$$J_3 \sim (\pi/T) E^{-1/2} - 2(E)^{-1} i$$

$$J_4 \sim (\pi B - 2T) E^{-1} - \pi E^{-1/2} i$$

For large values of E, the exact constants C and D become

$$C \sim N\pi i / B(B+T)$$

$$D \sim \left\{ N\pi / B(K_0 - iT) \right\} \left\{ 1 + (A/4\pi) (\pi/T(B+T)) \right\}$$

APPENDIX II

Using Born trial functions $f_{01} = (K_0^2 | k_1 k_2); (K_0^2 = B^2 + E)$, and $f_{02} = (K_1 K_2; k_1 k_2)$, $(K_1^2 + K_2^2 = E)$, in the Schwinger variational principle of section (2.6) yields the following values for the constants C and D.

$$C = \left[N\pi i / B(B+T) \right] \left[1 - (A/4\pi) J_1 i + (A/4\pi) (BJ_2 + iJ_3) \delta + (A/4\pi) (J_4/T) h \right] \Delta^{-1}$$

$$D = \left[N\pi / B(K_0 - iT) \right] \left[1 - (A/4\pi) J_1 i + (A/4\pi) (BJ_2 + iJ_3) \epsilon + (A/4\pi) (J_4/T) \zeta \right] \Delta^{-1}$$

$$\Delta = \left[1 - (A/4\pi) J_1 i + (A/4\pi) (BJ_2 + iJ_3) (B+T) (2T)^{-1} - (A/4\pi) (J_4/T) (K_0^2 + T^2) (2T)^{-1} (B+T)^{-1} \right] \\ \left[1 - (A/4\pi) J_1 i - (A/4\pi) (BJ_2 + iJ_3) (B+T) (K_0 - iT)^{-1} (\beta/i\alpha) + (A/4\pi) (J_4/T) (\gamma/\alpha) \right]$$

where

$$\alpha = \frac{1}{K_1 + iT} \frac{|K_2|}{|K_2| + Bi} - \frac{i(B+T)}{K_0 - iT} \left(\frac{1}{K_2 + iT} + \frac{Bi}{(|K_2| + Bi)(|K_2| - iT)} \right)$$

$$\beta = - \frac{1}{K_1 + iT} \frac{|K_2|}{|K_2| + Bi}$$

$$\gamma = - \left(\frac{1}{K_2 + iT} + \frac{Bi}{(|K_2| + Bi)(|K_2| - iT)} \right)$$

$$\epsilon = \frac{B+T}{K_0 - iT} \left(i \frac{\beta}{\alpha} + \frac{K_0 + iT}{2T} \right)$$

$$h = \frac{1}{B+T} \left(\frac{\gamma(B+T)}{\alpha} - \frac{K_0^2 + T^2}{2T} \right)$$

$$\epsilon = \frac{B+T}{K_0 - iT} \left(\frac{K_0 - iT}{2T} + \frac{i\beta}{\alpha} \right)$$

$$\zeta = - \frac{K_0 - iT}{B+T} \left(\frac{i\beta}{\alpha} + \frac{K_0 + iT}{2T} \right)$$

$$K_1^2 + K_2^2 = E \text{ and } K_0^2 = B^2 + E.$$

Three limiting cases may be immediately evaluated.

Case 1 — $K_2^2 \sim E$, K_1 small and E large.

Then $C \sim N\pi i / B(B+T)$ and

$$D \sim N\pi / B(K_0 - iT).$$

These are the Born results.

Case 2 — $K_1^2 \sim E$, K_2 small and E large .

Then

$$C \sim \frac{N\pi i}{B(B+T)} \left[1 - \frac{A}{4\pi} \frac{\pi}{T} \frac{(B \pm B) - T}{T^2 + (B+T) \{(B \pm B) - T\}} \right]^{-1}$$

and

$$D \sim \frac{N\pi}{B(K_0 - iT)} \left[1 - \frac{A}{4\pi} \frac{\pi}{T} \frac{(B \pm B) - T}{T^2 + (B+T) \{(B \pm B) - T\}} \right]^{-1}$$

The plus sign in $(B \pm B)$ is to be associated with positive values of K_2 and the minus sign with negative values of K_2 .

These results do not reduce to the Born results unless $T = 2B$ and K_2 is taken positive.

Case 3 — $K_1^2 = K_2^2 \sim E/2$; E large. The results for C and D are those of the first case considered.

APPENDIX III

An Alternative Proof of the Relation Between the Hulthén-Kohn and Schwinger Variational Principles

$$I \{v_i, v\} = \lim_{E' \rightarrow E} \left(v_i(E'), \{H - E\} v(E) \right) \quad (1)$$

H in (1) represents the Hamiltonian operator associated with the problem under consideration. The Hamiltonian H may be resolved in the following way:

$$H = H_0 - E + V$$

Here the operator $H_0 - E$ may be considered to represent the system when the component parts do not interact, i.e., in the region in which V is negligible. The Schroedinger equation is then

$$(H_0 - E + V) f(E) = 0 \quad (2)$$

or

$$(H_0 - E) f(E) = -Vf(E). \quad (3)$$

Equation (3) may be solved symbolically and the solution is

$$f(E) = f_0(E) - \{H_0 - E - i\alpha\}^{-1} Vf(E), \quad (4)$$

where $f_0(E)$ satisfies

$$(H_0 - E) f_0(E) = 0$$

and satisfies the initial conditions of the problem. Equation (4)

represents the solution $f(E)$ as an incident wave plus outgoing waves.

Another solution of (3) which represents an incident wave plus incoming waves is given by

$$f_i(E) = f_{oi}(E) - (H_0 - E + i\alpha)^{-1} V f_i(E), \quad (5)$$

where $f_{oi}(E)$ is any solution of

$$(H_0 - E) f_{oi}(E) = 0. \quad (6)$$

Multiply equations (4) and (5) by V , then these equations may be expressed as

$$Vf_0(E) = Vf(E) + V \{H_0 - E - i\alpha\}^{-1} Vf(E) \quad (7)$$

$$= (V + V \{H_0 - E - i\alpha\}^{-1} V)f(E) \equiv K f(E)$$

and

$$Vf_{0i}(E) = (V + V \{H_0 - E + i\alpha\}^{-1} V) f_i(E) \equiv K' f_i(E). \quad (8)$$

The definitions of the operators K and K' immediately lead to the relation that

$$(x, Ky) = (K'x, y) \quad (9)$$

i.e., that K' is the hermitian adjoint of K . Therefore from (7) and (8)

$$\begin{aligned} (f_i(E), Vf_0(E)) &= (f_i(E), Kf(E)) = (K'f_i(E), f(E)) \\ &= (Vf_{0i}(E), f(E)). \end{aligned} \quad (10)$$

Take the following trial function for $v(E)$

$$v(E) = f_0(E) - \left\{ (f_{0i}, Vf) / (f_{0i}, Vg) \right\} \{ (H_0 - E - i\alpha)^{-1} Vg \} \quad (11)$$

where g is an arbitrary function. When g is equal to f then $v(E) = f(E)$ from (4). Substitute (11) into (1).

(12)

$$\begin{aligned} I \{v_i, v\} &= \lim_{E' \rightarrow E} \left(v_i(E'), \{H_0 - E + V\} \left[f_0(E) - \left\{ (f_{0i}, Vf) / (f_{0i}, Vg) \right\} \{ (H_0 - E - i\alpha)^{-1} Vg \} \right] \right) \\ &= \lim_{E' \rightarrow E} \left(v_i(E'), Vf_0(E) - \left\{ (f_{0i}, Vf) / (f_{0i}, Vg) \right\} \{ Vg + V(H_0 - E - i\alpha)^{-1} Vg \} \right) \\ &= \left(v_i(E), Vf_0(E) - \left\{ (f_{0i}, Vf) / (f_{0i}, Vg) \right\} Kg \right) \end{aligned}$$

where the definition of K of equation (7) has been used. The limit may be taken in (12) because the potential function is a well behaved function and the limiting process may be interchanged with the operation defined by the inner product. Then, omitting the dependence of the quantities on E ,

$$\begin{aligned} I \{v_1, v\} &= I' \{v_1, g\} = (v_1, Vf_0) - (f_{01}, Vf)(v_1, Vf_0) \lambda \{v_1, g\} \\ &= (v_1, Vf_0) \left[1 - (f_{01}, Vf) \lambda \{v_1, g\} \right] \end{aligned} \quad (13)$$

where

$$\lambda \{v_1, g\} \equiv (v_1, Kg) / (v_1, Vf_0)(Vf_{01}, g) \quad (14)$$

Equation (14) is the expression associated with the Schwinger variational principle.

Consider the variation of (13) about the solution of (4) and (5).

$$\begin{aligned} \delta I \left\{ v_1, v \right\}_{\substack{v=f \\ v_1=f_1}} &= \delta I' \left\{ v_1, g \right\}_{\substack{g=f \\ v_1=f_1}} = \left[(\delta v_1, Vf_0) - (f_{01}, Vf)(v_1, Vf_0) \delta \lambda \{v_1, g\} \right. \\ &\quad \left. - (f_{01}, Vf) \lambda \{v_1, g\} (\delta v_1, Vf_0) \right]_{\substack{g=f \\ v_1=f_1}} \\ &= -(f_{01}, Vf)^2 \delta \lambda \left\{ v_1, g \right\}_{\substack{g=f \\ v_1=f_1}} \end{aligned} \quad (15)$$

For from (10) and (14),

$$(f_1, Vf_0) = (Vf_{01}, f) \text{ and } \lambda \{f_1, f\} = 1/(Vf_{01}, f) \text{ respectively.}$$

Equations (13) and (15) establish the relations sought.

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